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A WORKBOOK OF SCREENING TECHNIQUES FOR ASSESSING IMPACTS OF TOXIC AIR POLLUTANTS



A Workbook Of Screening Techniques For Assessing Impacts Of Toxic Air Pollutants

by.

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1.0 INTRODUCTION

This workbook provides a logical approach to the selection of appropriate screening techniques for estimating ambient concentrations due to various toxic/hazardous pollutant releases. Methods used in the workbook apply to situations where a release can be fairly well defined, a condition typically associated with non-accidental toxic releases. The format of this workbook is built around a series of scenarios which may be considered typical and representative of the means by which toxic chemicals become airborne. In addition, suggestions are provided for modeling less typical cases.

Screening techniques are simplified calculational procedures designed with sufficient conservatism to allow a determination of whether a source: 1) is clearly not an air quality threat or 2) poses a potential threat which should be examined with more sophisticated estimation techniques or measurements. Screening estimates obtained using this workbook represent maximum short-term ground level concentration estimates from a meteorological perspective. If the screening estimates demonstrate that during these conditions the ground level concentrations are not likely to be considered objectionable, further analysis of the source impact would not be necessary as part of the air quality review of the source. However, if screening demonstrates that a source may have an objectionable impact, more detailed source impact analysis would be required using refined emissions and air quality models.

Methods used in this workbook should be applied with caution. Techniques for estimating emissions are evaluated and revised on a continuing basis by EPA. Thus the user should consult with EPA on the most recent emission models and emission factors. Meteorological methods presented in this report reflect guidance published elsewhere, and in particular the Procedures for Evaluating Impact of Stationary Sources that includes the PC-based model SCREEN (1988b) and the Guideline on Air Quality Models (Revised) (1986) and Supplement A

(1987). The Regional Modeling Contact should be consulted as to the present status of guidance in air quality modeling.

The workbook is organized into six sections and six supporting Section 2 discusses selection of screening techniques and the general approach to using the workbook. Users are advised to consult this section both for releases explicitly presented in the workbook and for less typical releases. The section also considers assumptions, limitations and conservatism of estimates. Section 3 describes the support data (i.e., meteorological data and chemical and physical parameters) needed for making estimates. Section 4 helps the user identify applicable release scenarios and determine release and emission rates. In this workbook 18 release scenarios have been selected to represent situations likely to be encountered. Section 5 of the report guides the user through all the steps required for making atmospheric dispersion estimates once atmospheric emissions contaminant characteristics are known. Section 6 provides an example of the emission and associated dispersion estimation methods for each specific release scenario.

Appendix A discusses currently available sources for obtaining emission factors that can be used for some of the scenarios. Appendix B provides a glossary of terms applicable to air toxics modeling. Appendices C and D contain flow diagrams to be used as a guide in Sections 4 and 5 for selecting applicable emission and dispersion calculation methods. Appendix E presents methods for converting concentrations to different averaging times. Appendix F provides some useful unit conversion factors applicable to the workbook. Appendix G provides methods for calculating dispersion parameters as an alternative to using graphical methods.

This workbook supersedes information in EPA Report EPA-450/4-86-11, Some Applications of Models to Air Toxics Impact Assessments.

2.0 SELECTION OF SCREENING TECHNIQUES FOR TOXIC AIR CONTAMINANTS

This workbook attempts to account for many of the scenarios expected to produce toxic chemical releases to the atmosphere.

2.1 Release Categorization

Selection of appropriate techniques for screening estimates requires categorization of the toxic chemical release of interest. There are three overlapping categories which should be considered when defining problems for screening:

- Physical State Gaseous releases to the atmosphere can, in general, be simulated using techniques developed for criteria air pollutants unless the gas is dense, is highly reactive, or rapidly deposits on surfaces. Additional source modeling must be performed if the release is liquid, aerosol or multi-phased to determine the state of the material as it becomes available for dispersion in air.
- 2) Process/Release Conditions Knowledge of the circumstances under which chemicals are released helps to determine both state and dispersive characteristics. For example, location of a leak in a pressurized liquefied gas storage tank will determine if a release is liquid or gas and if source modeling is required prior to dispersion estimates.
- 3) Dispersive Characteristics Techniques for pollutant dispersion estimates are categorized by terms such as instantaneous versus continuous, or point versus area or volume releases. To complete dispersion estimates, this final characterization is required at some point in concentration calculations.

The primary emphasis in this workbook is to provide the user with screening techniques for estimating short-term, ground level concentrations of toxic chemicals released to the atmosphere. However, in order to do this, the workbook also provides assistance to the user in formulating the release conditions. In framing each problem, the user must reason the path required to complete the concentration estimate.

2.2 Limitations and Assumptions

Methods included in this workbook are intended to provide simplified, conservative dispersion estimates for situations which may represent extremely complex release scenarios. As such, the methods are limited in their applicability. Some of these limitations are as follows:

- Screening techniques provided are intended for use on small to mid-scale non-accidental releases.
- All techniques assume that the toxic air contaminant is nonreactive and non-depositing. Thus these screening methods are not applicable for reactive gases and settleable particles.
- Conditions resulting in worst case concentrations cannot be uniquely defined in instances where gases released are denser than air or where meteorological conditions affect source estimates. For example, in the case of evaporation, the highest source rates are related to high wind speeds. High wind speeds, however, result in more dilution which acts to lower concentrations in air.
- Time dependent emissions cannot be simulated with a simple screening technique. Techniques provided assume steady releases for a specified period.
- Methods are not provided for the following phenomena:
 - heavy gas releases influenced by obstructions to flows
 - non-vertical jet releases of heavy or passive gases
 - the influence of aerosol evaporation, deposition, surface or radiational cloud heating and exothermic or endothermic reactions on dispersing clouds
- All release calculations assume thermodynamically ideal conditions for gas and liquid flows.
- Pasquill-Gifford dispersion parameters for continuous plumes (Turner, 1970) are assumed to represent hourly average conditions.
- Building wake effects calculations are based on methods used in the Industrial Source Complex Model (EPA, 1987c) and cavity calculations are based on methods in Procedures (EPA, 1988b). Simple rectangular building geometries are assumed in both cases. When a selection of wake effects is made, calculations are not performed for receptors within three building heights downwind.
- Complex and elevated terrain effects are not considered.

- Sources in rural and urban settings can use the same procedures presented here. Dispersion parameters for urban settings are not presented. They may be obtained from other EPA publications.
- Screening techniques are applicable to short-term concentration estimates.

2.3 Technique Selection and Use

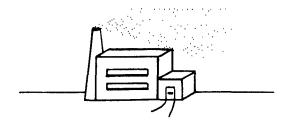
Eighteen most prevalent release scenarios were selected for this workbook and are grouped in Table 2-1 according to three categories: particulate matter, gases and liquids. For some of the release scenarios, subcategories have been added. Table 2-1 also provides a convenient look-up table to indicate relevant sections in this report that are associated with each release scenario. Figure 2-1 provides a graphical illustration of each release scenario. Appendix C guides the user through techniques for estimating release and emission rates. Appendix D guides the user in selecting the atmospheric dispersion estimates for these scenarios. The first step in analyzing any scenario is, therefore, to consult the appropriate release flowchart in Appendix C.

Steps in using the workbook are as follows:

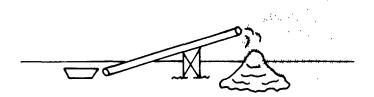
- 1. Select the release scenario from Figure 2-1 and Table 2-1 which most closely resembles the release of concern. Release descriptions provided in the report sections and noted in the table provide selection guidance.
- 2. Follow the instructions given in the report section describing the release of concern. The flowchart referenced either guides the user through emission calculations in Section 4 or indicates that emission estimates can be obtained from a separate source of emission factors (Appendix A).
- 3. The final step of the applicable release flowchart indicates the appropriate dispersion flowchart in Appendix D which guides the user in determination of ambient concentrations. The user should proceed to the flowchart keeping in mind the dispersion modeling category specified for the release scenario of concern in Table 2-1 (i.e., instantaneous or continuous emissions from a point, area, or volume source). The dispersion model category is used at a decision point in the dispersion flowchart.

Initial Form of Release	Release Type	Modeling Category*	Emission Section	Emission Flowchart	Initial Dispersion Flowchart	Example Section
Particulate Matter	Stack Fugitive Dust Duct Failure	CP CA IV	4.1.1 4.2 4.3	G G-2 G-3 G-3	D-2 D-4 D-6	6.2 6.3
Gases	Flares Stacks, Relief Valves, Vents Gas Leaks: Tanks, Pipes, Pumps, Compressors Stacks, Relief Valves, Vents Multiple Fugitive Emissions Land Treatment Emissions Municipal Solid Waste Landfill Emissions Pesticides/Herbicides Equipment Openings	មិខិមិ ដូ ខិ ទីទីទី≥ិ	4.4 4.5 4.5 6.7 4.9 4.10	C-4 C-5 C-5 C-9 C-10 C-12	D-7 D-1 D-1 D-4, D-5 D-4 D-4 D-4	6.4 6.5 6.5 6.7 6.8 6.9 6.10
Liquids	Surface Impoundments (Quiescent) Surface Impoundments (Aerated) Continuous Relief Valve Discharge (two phase), Two Phase Tank Leaks Instantaneous Relief Valve Discharge (two phase) Liquid Leaks - Pipes (non-pressurized, low volatility): continuous, finite Liquid Leaks - Tanks (low volatility) Liquid Leaks - Pipes (high volatility)	ଶ୍ରିଷ ଧା ଶ୍ରୀଷ	4.12 4.12 4.13 4.14 4.15	C-13 C-14 C-15 C-15 C-16 C-17	D-4 D-4 D-4 D-4	6.12 6.12 6.13 6.14 6.15 6.15
		යි	4.18	C-19	D-1	6.18

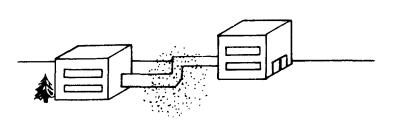
^{*} C - Continuous P - Point A - Area I - Instantaneous V - Volume



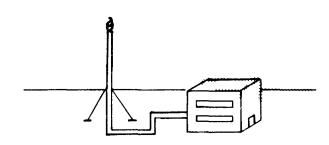
STACK RELEASES OF GASES OR PARTICLES (4.1.1, 4.1.2)



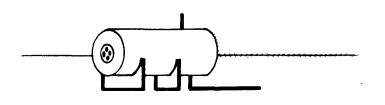
FUGITIVE DUST EMISSIONS (4.2)



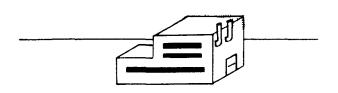
PARTICULATE MATTER
DUCT FAILURES (4.3)



FLARE EMISSIONS (4.4)

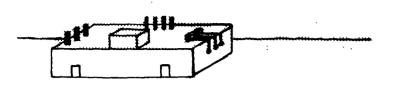


GAS LEAKS (4.5)



INSTANTANEOUS
GASEOUS EMISSIONS (4.6)

FIGURE 2-1. RELEASE SCENARIOS (Section Number in Parentheses)



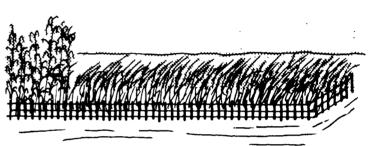


MULTIPLE FUGITIVE EMISSIONS (4.7)

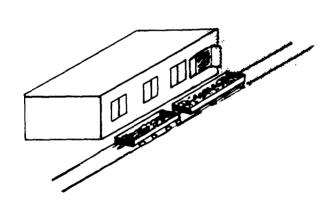
LAND TREATMENT (4.8)



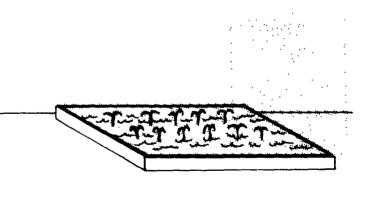




PESTICIDES/HERBICIDES (4.10)



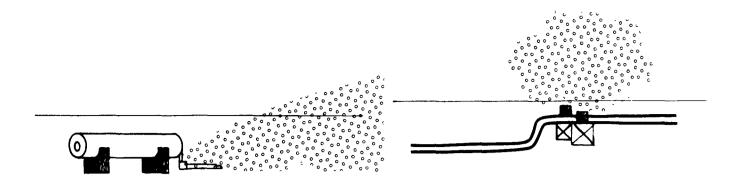
EQUIPMENT OPENING (4.11)



SURFACE IMPOUNDMENTS (4.12)

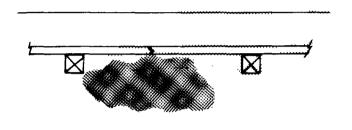
FIGURE 2-1. RELEASE SCENARIOS (Continued)

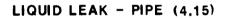
(Section Number in Parentheses)

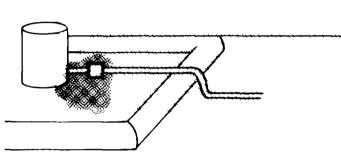


RELIEF VALVE - CONTINUOUS (4.13)

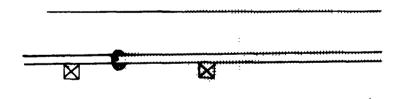
RELIEF VALVE - INSTANTANEOUS (4.14)



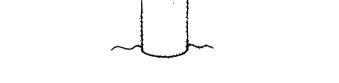




LIQUID LEAK - TANK (4.16)



HIGH VOLATILITY PIPE LEAKS (4.17)



HIGH VOLATILITY TANK LEAKS (4.18)

FIGURE 2-1. RELEASE SCENARIOS (Continued)

(Section Number in Parentheses)

4. The concentrations obtained are representative of the averaging times identified. Procedures to convert concentrations to other averaging times are described in Appendix E.

2.4 Determining Maximum Short-Term Ground Level Concentration

In modeling air toxic releases, a reasonable degree of assurance is needed that the maximum short-term ground level concentration estimate from a meteorological perspective is obtained. This maximum concentration is selected from those concentrations calculated using the range of stability classes and wind speeds in Table 2-2.

The first choice is to use all six stability classes and their associated wind speeds. To reduce the number of calculations, the second choice is to use a subset of these meteorological conditions associated with the emission release condition for the scenario of concern. While these subsets will generally provide maximum concentration estimates, the user may wish to use the entire range of conditions in Table 2-2 to provide greater assurance that the maximum concentration is always calculated.

A. Continuous Passive Releases

Concentration estimates for continuous passive (non-dense) releases should be made by using the applicable procedures in Table 2-3.

B. Instantaneous Passive Releases

Concentration estimates for instantaneous passive (non-dense) releases should be made for the following conditions:

- I. Ground level releases: use stability class F and 1 m/s wind speed
- II. Elevated releases: use stability classes A, C, and F each with 1 m/s wind speeds. Calculate concentrations at the greater of the distance at which the vertical dispersion coefficient, $\sigma_{\rm Z}$, equals $H/\sqrt{2}$ (where H = release height) or the fenceline distance. Select the maximum of these concentration estimates.

TABLE 2-2
WIND SPEED AND STABILITY CLASS COMBINATIONS

				10-m	Wind (m/s)		đ		
Stability Class	1	2	3	4	5	8	10	15	20
A (very unstable)	*	*	*						
B (moderately unstable)	*	*	*	*	*				
C (slightly stable)	*	*	*	*	*	*	*		
D (neutral)	*	*	*	*	*	*	*	*	*
E (slightly stable)	*	*	*	*	*				
F (moderately stable)	*	*	*	*					

TABLE 2-3

CALCULATION PROCEDURES FOR USE WITH VARIOUS EMISSION HEIGHTS (CONTINUOUS RELEASES)

Height of Emission	Stability Classes	Wind Speed (m/s)*
I. Stack Height > 50 m**	A	1 and 3
- <u>-</u>	C	1, 3, 5, 8 and 10
II. 10 m < stack height < 50 m**	A	1 and 3
-	C	1, 3, 5, 8 and 10
	F	1, 3 and 4
II. Stack height < 10 m and some	С	1, 3, 5, 8 and 10
plume rise	F	1, 3 and 4
<pre>IV. Stack height < 10 m and no plume rise; all ground level sources</pre>	F	1
V. Wake effects exist	С	1, 3, 5, 8 and 10
	F	1, 3 and 4
Cavity effects exist ***	- -	10 for critical spee 1 for dilution in concentration equation

^{*} Use 10 m wind speed adjusted to stack height using the equation in Section 3.1.1 with the exponents as shown in Table 3-1.

^{**} For these sources, the user should determine the distance to fenceline, X_{fc} , and the distance to final plume rise, X_f . If:

 X_{fc} > X_f final plume rise is used. (The distance to the maximum concentration is found at $\sigma_z = H/\sqrt{2}$. Where, H = release height, and σ_z = vertical plume dispersion). For each stability class, the distance is determined using a wind speed of 1 m/s. The greater of this distance or the distance to the fenceline is used in the estimate.

 $[\]rm X_{fc}$ < $\rm X_{f}$ transitional plume rise is used, and the calculations must iterate over several distances from $\rm X_{fc}$ to $\rm X_{f}$, usually at 100 m intervals.

^{***} Cavity effects are assumed independent of stability classes.

C. Dense Gas Releases

- I. For a continuous dense gas release, the maximum ground level concentration usually occurs under light wind speed, stable atmospheric conditions, but this may vary depending upon receptor location relative to initial dilution and gravitational spreading of the heavy gas cloud (spreading is a function of initial release size and density). Because of the complexity of making dense gas calculations, hand calculations are impractical. The use of the EPA Relief Valve Discharge (RVD) model is recommended (see Section 5.6.3). This model is not dependent on stability. After running the model using a range of wind speeds, the maximum concentration is estimated at the farther of the plume touchdown distance and the distance to the fenceline.
- II. For instantaneous dense gas releases, a simple model is provided in Section 5.6.2. As a conservative approximation, elevated releases should be simulated using the ground level model. The maximum concentration release is obtained by assuming Gaussian dispersion and using stability class F with 1 m/s wind speed.

The user should carefully examine each release scenario and use the appropriate approach from those listed above to determine maximum concentrations. There is no universal approach to use for all cases. However, Table 2-4 summarizes approaches that may be used for the scenarios described in the workbook.

		Source		Release Type	Туре		ecomm	Recommended Approach for Obtaining	Appro m Con	ach :	or O	otain	ing	1
Release Scenario	Point	Area	Volume	Passive	Dense	A*	A	A III	A VI	∢>	1 I	B II	υH	CII
1. Continuous Particulate and Gaseous Releases from Stacks	××			×	×	×	×			×			×	
2. Continuous Releases of Fugitive Dust		×		×					×					
3. Ducting Failures with Dust Releases	×										×			
4. Flare Emissions	×			×		×	×							
5. Continuous Gaseous Leaks from Tanks/Pipes	××			×	×				×				×	
6. Instantaneous Gaseous Releases from Stacks	××			×	×							×		×
7. Multiple fugitive Continuous Gaseous Emission Sources		×	×	××					××					
8. Continuous Gaseous Emissions from Land Treatment		×		×					×					
9. Continuous Emissions from Municipal Solid Waste Landfills		×		×					×					
10. Continuous Emissions of Pesticides and Herbicides		×		×					×					
ll. Instantaneous Emissions Due to Equipment Openings	×	×	×	×	×						×		^	×
12. Evaporation from Quiescent or Aerated Surface Impoundments		×		×					×					
13. Continuous Relief Valve Discharges (Two-Phase Flow)	××			×	×				×				×	
14. Instantaneous Relief Valve Discharges (Two-Phase)	××			×	×				×					×
15. Low Volatility Liquid Leaks from Pipes		×		×					×					
16. Low Volatility Liquid Leaks from Tanks		×		×					×					
17. High Volatility Liquid Leaks from Pipes	×			×					×					
18. High Volatility Liquid Leaks from Tanks	×			×					×					- 1

* A – continuous/passive B – instantaneous/passive C – dense gas

3.0 SUPPORT DATA FOR SCREENING ESTIMATES

Simulations for air toxic releases require information on the meteorological conditions at the time of release as well as physical and chemical parameters describing the materials being released.

3.1 Meteorological Data

Computational procedures for estimating concentrations require data on wind speed and direction, temperature and atmospheric pressure. These data are normally collected at National Weather Service stations and some military installations on an hourly basis. Stability and turbulence parameters can be estimated from cloud data as described below. A record of these is available from the National Climatic Data Center, Asheville, North Carolina. Meteorological data are sometimes recorded at air quality monitoring sites at existing plants. The use of the on-site data with proper quality assurance procedures as described in On-site Meteorological Program Guidance for Regulatory Modeling Applications (EPA, 1987d) is preferred.

3.1.1 Wind Speed and Direction

Wind speed and direction data are required to estimate short-term peak concentrations. Wind speed is used to determine (1) plume dilution, (2) plume rise and (3) mass transfer in evaporation models. These factors, in turn, affect the magnitude of, and distance to, the maximum ground-level concentration.

Most wind data are collected near ground level. The wind speed at release height can be estimated by using the following power law equation:

$$u = u_1 \left(\frac{h}{z_1}\right)^p$$

where:

- u = the wind speed (m/s) at release height h (m),
- u_1 = the wind speed at the anemometer height z_1 (m), and
- p = the stability-related exponent from Table 3-1.

TABLE 3-1
WIND PROFILE EXPONENT AS A FUNCTION OF ATMOSPHERIC STABILITY

	Rural	
Stability Class	Exponent	
A	0.07	
 В	0.07	
C	0.10	
D	0.15	
E	0.35	
F	0.55	

The wind direction is an approximation for the direction of transport of the plume. The variability of the direction of transport over a period of time is a major factor in estimating ground-level concentrations averaged over that time period.

3.1.2 Stability and Turbulence

Stability categories, as depicted in Tables 3-1 and 3-2, are indicators of atmospheric turbulence. The stability category at any given time depends upon thermal turbulence (caused by heating of the air at ground level) and mechanical turbulence (a function of wind speed and surface roughness). Stability is generally estimated by a method given by Turner (1970), which requires information on solar elevation angle, cloud cover, cloud ceiling height, and wind speed (see Table 3-2).

The solar elevation angle is a function of the time of year and the time of day, and is presented in charts in the Smithsonian Meteorological Tables (List, 1968). The hourly weather observations of the National Weather Service

TABLE 3-2
KEY TO STABILITY CATEGORIES

		Day		Night*	
Surface Wind	Incomin	g Solar Radia	tion**	Thinly Overcast	
Speed at a	(Insolation)			or	< 3/8
Height of 10m	Strong	Moderate	Slight	> 4/8 Low	Cloud
(m/sec)				Cloud Cover	Cover
< 2	A	A-B	В	_	_
2-3	A-B	В	C	E	F
3-5	В	B-C	C	D	E
5-6	С	C-D	D	D	D
> 6	C	D	D	D	D

The neutral class (D) should be assumed for all overcast conditions during day or night.

- * Night is defined as the period from one hour before sunset to one hour after sunrise.
- ** Appropriate insolation categories may be determined through the use of sky cover and solar elevation information as follows:

Sky Cover	Solar Elevation Angle > 60°	Solar Elevation Angle ≤ 60° But > 35°	Solar Elevation Angle ≤ 35° But > 15°
4/8 or Less or Any Amount of High Thin Clouds	Strong	Moderate	Slight
5/8 to 7/8 Middle Clouds (7000 feet to 16,000 foot base)	Moderate	Slight	Slight
5/8 to 7/8 Low Clouds (less than 7000 foot base)	Slight	Slight	Slight

include cloud cover, cloud ceiling height, and wind speed. Methods for estimating atmospheric stability categories from on-site data are provided in EPA modeling quidelines.

Friction velocity (u_*) represents mechanical turbulence due to wind flow over the surface and is used in calculating release Richardson number. Friction velocity is a function of stability, decreasing with increasing stability. An approximation of friction velocity under neutral stability conditions and assuming a roughness length of 1 cm is:

$$u_{\perp} = 0.06u$$

where u is the wind speed (m/s) at a height of 10 m.

3.1.3 Temperature

Ambient air temperature must be known in order to calculate the amount of rise of a buoyant plume and to calculate evaporation rates.

3.1.4 Atmospheric Pressure

Atmospheric pressure data are used in calculating gas and liquid release rates from storage and process vessels and pipes.

3.2 Chemical and Physical Parameters

Numerous chemical and physical properties of chemicals and spill substrates are required to use some of the emission estimation techniques presented. A list of typical physical and chemical properties and their typical units as used in this workbook is shown in Table 3-3. The complexity and diversity of chemical and physical behavior of the many air toxic substances make it critical that the correct input parameters are obtained. These parameters can be found in compendiums of physical and chemical characteristics. Three of the more comprehensive sources of information are:

TABLE 3-3

TYPICAL PHYSICAL AND CHEMICAL PROPERTY PARAMETERS USED IN EMISSION MODELING

Parameter Name	Typical Units
Boiling point at ambient pressure	°K
Specific heat of liquid	
- at constant pressure	cal/g-mole °K
- at constant volume	cal/g-mole °K
Specific heat of vapor	
- at constant pressure	cal/g-mole °K
- at constant volume	cal/g-mole °K
Molecular weight	g/g-mole
Latent heat of evaporation	cal/g-mole
Vapor pressure	atm
Vapor density	g/m ³
Liquid density	g/m ³
Specific gravity (S.G.)	
Constituent diffusivity	
(diffusion coefficient)	
- in air	cm ² /s
- in water	cm ² /s
- in oil	cm ² /s
Henry's Law constant	atm-m ³ /g-mole
Solubility in water	g-mole/m ³
Net heating value	cal/g-mole

Beilstein, 1987: <u>Handbook of Organic Chemistry</u>, Springer-Verlag, New York.

Green, D., 1984: <u>Perry's Chemical Engineer's Handbook</u>, Sixth Edition, McGraw-Hill, New York.

Verschueren, K., 1983: <u>Handbook of Environmental Data on Organic Chemicals</u>. Van Nostrand Reinhold Company, New York.

The user should be cautioned that a characteristic "constant" used in modeling may have different values depending on the reference from which the parameter was obtained.

4.0 SCENARIOS AND TECHNIQUES FOR RELEASE AND EMISSIONS ESTIMATES

Techniques for estimating air toxics emissions must be capable of treating a large variety of potential release scenarios. This section is intended to help the user identify the applicable release scenario and determine release and emission rates and to guide the user through remaining calculations to arrive at a concentration estimate. Eighteen release scenarios are presented in this workbook. Descriptions of similar releases are provided, and the user is advised to review these descriptions if an obvious choice is not apparent in Table 2-1.

Since so many varied processes and sources have the potential for toxic chemical releases, the eighteen scenarios cover a small percentage of possible release, emission, and dispersion combinations. Techniques in this section estimate emissions to the atmosphere after providing guidance on release calculations. In these cases and in all other applications, the characterization of emissions is a critical step which is best met through a complete and accurate measurement program. In practical applications, measured data are seldom available and the user is left to techniques such as those presented in this section, data from existing inventories, emission factors, or process specific material balance estimates.

Some of the numerous sources of existing data are permit and registration files, technical literature, and SARA Title III reporting forms. A new data source summarizing regulatory data is the National Air Toxics Information Clearinghouse (NATICH) and Data Base. Information on NATICH is available through EPA Regional Air Toxics Contacts and:

Pollutant Assessment Branch (MD-12) U.S. Environmental Protection Agency Research Triangle Park, NC 27111 (919) 541-0850 FTS 629-0850 For some sources, mass balances are used to estimate releases when conservative assumptions concerning quantities of input and output streams are made. The amounts entering and/or leaving a process can be measured or estimated. A mass balance can then be performed on the process as a whole or on the subprocess. For processes where material reacts to form a product or is significantly changed, use of mass balance may be too difficult for estimating emissions and the use of emission factors may be more appropriate.

When measured or plant specific data are unavailable, the user is advised to review emission factors developed for specific processes. Appendix A provides a description of sources of emission factors.

4.1 Continuous Particulate and Gaseous Releases from Stacks

Similar Releases: Continuous emissions of particulate matter and gases from building vents, vertical stacks and pipes, or conventional point sources when emission flowrates and temperature are known. Combustion sources, chemical reactors, and some process vents are typical emission sources that emit pollutants through stacks. These releases may also be due to a process failure such as a rupture disk release or failure of control equipment.

4.1.1 Particulate Matter

Continuous emissions of particulate from stacks are analyzed beginning with Flowchart C-1. EPA recommends that emission rates from such sources be determined through source testing using EPA Reference Methods (40 CFR Part 60 Appendix A) or process calculations. If source-specific emissions are not available, representative emission factors can be substituted. Emission factors are available for individual toxic compounds (Appendix A, items 1, 2, and 3). Otherwise, factors determined by compiling extensive source test results using EPA Reference Methods are reported in AP-42. Toxic components of emissions can be determined using the Air Emission Species Manual, Volume II, Particulate Matter Species Profiles (Appendix A, item 4).

Once emissions of the toxic pollutants are determined, this release scenario represents a case for which ground level concentration estimates can be made using specific dispersion calculations outlined in Flowchart D-2 (Appendix D). Specific equations to be applied can be found in the report sections referenced in each flowchart. For point sources, calculations begin with determining if cavity or wake analysis is applicable as outlined in Flowchart D-2. If the plume is in the cavity or the wake region, then cavity and wake impacts must be determined. If the plume is outside of the cavity or wake regions, then basic point source techniques are applied as shown in

Flowchart D-3. Section 6.1 provides an example of this scenario. Maximum concentrations are obtained as shown in Table 2-3.

4.1.2 <u>Gases</u>

Continuous emissions of gases from stacks are analyzed beginning with Flowchart C-5. Emission factors are available for individual toxic compounds (Appendix A, items 1, 2, and 3). Otherwise, total VOC emission rates can be obtained from AP-42 in a similar manner as discussed in Section 4.1.1. Toxic components of these emissions can be determined using the Air Emission Species Manual, Volume I, Volatile Organic Compound Species Profiles (Appendix A).

Dispersion techniques for continuous gaseous emissions (Flowchart D-1) use similar techniques to modeling particulate emissions except that cloud density calculations are used to determine if dense gas effects may be applicable. If the gas is not dense, passive point source techniques apply (Flowchart D-2).

4.2 Continuous Releases of Fugitive Dust

<u>Similar Releases</u>: Any fugitive dust from process losses, generation by mechanical action in material handling or windblown dust.

These fugitive dust releases are generalized area emissions originating from a surface or collection of small, poorly quantified point sources. As indicated in Flowchart C-2, emissions are either user-specified or calculated with representative emission factors. Emission factors for fugitive dust emissions are typically found in AP-42 and are assumed to be independent of wind speed for this workbook. Toxic components can be determined using the Air Emission Species Manual, Volume II, Particulate Matter Species Profiles (Appendix A). Dispersion calculations for a continuous area source release are outlined in Flowchart D-4. For screening, particle settling is assumed to be insignificant. Virtual distances are determined for calculation of dispersion parameters, and concentrations are then calculated for the area source. Maximum concentration is obtained as shown in Table 2-4.

4.3 Ducting Failures With Dust Releases

<u>Similar Releases</u>: Instantaneous bursts of dust particles due to duct failure (e.g., pneumatic conveyor line failures), line disconnection, isolation joint failure, or other types of equipment openings.

Flowchart C-3 indicates that emission estimation techniques are not available for duct failures and user specification is required. Limited information on powder releases is available in the technical literature. Crude estimates of release amounts can be made based on transfer line rates and time for equipment shutdown and equipment capacity. Modeling for dispersion is shown in Flowchart D-6. If possible, the user should attempt to estimate the initial cloud dimension resulting from dilution due to the mechanical action of the release. If initial dilution can not be estimated by the user, conservative concentration estimates can be obtained using an instantaneous point source simulation (also Flowchart D-6). For screening, particle settling is assumed insignificant. Maximum concentration is obtained as shown in Table 2-4.

4.4 Flare Emissions

Flares are used as a control device for a variety of sources. As such, flares must comply with requirements specified in 40 CFR 60.18. Once emissions are vented through the flare, a minimum 98% reduction of all components of the flare must be achieved. Therefore, the user should calculate the process emissions that feed into a flare and multiply this number by 0.02 to achieve a conservative estimate of emissions emitted from the flare. After emissions are determined (Flowchart C-4), the user should calculate total plume rise from flares (Flowchart D-7). Flame tip height is calculated and added to the physical stack height to account for the distance between the flare outlet and the flame tip. Total heat release rate is calculated prior to use in buoyant plume rise equations. Continuous point source dispersion techniques are then used to determine dispersion parameters, buoyancy induced dispersion, and receptor concentrations (Flowchart D-3).

4.5 Continuous Gaseous Leaks from Tanks/Pipes

Similar Releases: Continuous gaseous emissions due to visible (usually) holes or openings in tanks, pipes, or flanges (e.g., at pipe connections, valves, pumps, and compressors).

Emissions due to continuous gaseous leaks from tanks or pipes can be estimated using the following procedures, as outlined in Flowchart C-6:

• Input:

P_a - atmospheric pressure (dynes/cm²)

Pt - tank or pipe pressure (dynes/cm²) A - hole or pipe area (cm²)

MW - molecular weight (g/g-mole)

 T_{t} - tank absolute temperature (deg. K) K - ratio of specific heat at constant pressure to specific

heat at constant volume

 $\rho_{\mathbf{V}}$ - vapor (gas) density (g/cm^3) $X_{\mathbf{i}}$ - mole fraction of each constituent in vapor

 Y_i - weight fraction of each constituent in vapor

• Limitations/Assumptions:

- Does not simulate time dependent release rates
- $C_{
 m d}$ coefficient of discharge range 0.6 1.0 (a value of 0.8 is used for screening)

• References:

- Hunsaker and Rightmire (1947)
- Fingas et al. (1986)

• Procedure:

1) If the gas is single component, proceed to step 2. For multicomponent gases, calculate the mean density of the pressurized gas and specific heats.

The mean density for calculations is:

$$\rho_{\mathbf{v}} = \rho_{\text{mean}} = \sum_{i=1}^{n} X_{i} \rho_{i}$$

Mean specific heats (calculate for both constant pressure, c_p , and constant volume, c_v)

$$c_{mean} = \sum_{i=1}^{n} Y_i c_i$$

The ratio of specific heats is:

$$K = \frac{C_{y \text{ mean}}}{C_{y \text{ mean}}}$$

A typical value of K at atmospheric pressure is 1.5.

2) Determine if the maximum (critical) release rate is to be calculated by evaluating the pressure ratio at the release point:

If:

f:
$$\frac{P_{t}}{P_{a}} \begin{cases} \left(\frac{K+1}{2}\right)^{\frac{K}{K-1}} & \text{use subcritical rate equation} \\ \frac{K}{2} \left(\frac{K+1}{2}\right)^{\frac{K}{K-1}} & \text{use critical rate equation} \end{cases}$$

A typical value for the right hand side is 2.0.

3) For critical flows, calculate:

Release rate (g/s)

$$q_v = C_d A \sqrt{\frac{K P_t P_v}{\left(\frac{2}{K+1}\right)} \frac{K+1}{K-1}}$$

4) For subcritical flows:

Release rate (g/s)

$$q_{v} = C_{d} A \sqrt{KP_{t} P_{v} \left(\frac{2}{K-1}\right) \left(\frac{P_{a}}{P_{t}}\right)^{K} - \left(\frac{P_{a}}{P_{t}}\right)^{K+1}}$$

• Jutput:

Vapor venting rate (q_v) in g/s for use in dispersion models.

After emissions are determined, point source dispersion techniques are applied (Flowchart D-1), including the determination of plume density and dense gas concentrations, if applicable. For non-dense gas releases, possible cavity or wake effects are examined (Flowchart D-2). Note, if the user cannot obtain reliable data to use in these equations, then the use of emission factors (Appendix A) is suggested as an alternative.

4.6 Instantaneous Gaseous Releases from Stacks

Similar Releases: Instantaneous gaseous vent releases or gas leaks and relief valve or rupture disk discharges which are of short duration (e.g., less than 5 minutes). These releases may arise from process upsets, chemical reactor process failures or equipment opening or purges.

Screening methods are not available for estimating emission rates, plume rise and downwash effects for this release type (Flowchart C-7). Emissions estimates for this scenario are generally process specific and must be specified by the user. Limiting estimates of emissions can be determined by considering the capacity of the source under consideration. For example, the maximum amount of gas released from a reactor would be the reactant or product amount.

Dispersion estimates can be obtained by applying the procedures outlined in Flowchart D-6. If the release is not dense (based on Richardson number criteria), instantaneous point source dispersion techniques are applied to obtain concentration estimates. If, however, the instantaneous puff is determined to be dense, concentrations are determined after including initial gravitational spreading. A coarse screening estimate for the effects of dense instantaneous gaseous releases can be performed assuming that the releases are undiluted and at ground level as indicated in Flowchart D-6.

Screening techniques are available for simulating only spreading and dispersion from a low momentum, ground-level dense release. Descent of elevated heavy gas clouds and high momentum associated with many instantaneous releases tend to provide significant initial dilution. This dilution acts to reduce concentrations and density. As a conservative estimate, elevated heavy gas dispersion from instantaneous releases is assumed to be at ground level.

4.7 Multiple Fugitive Continuous Gaseous Emission Sources

<u>Similar Releases</u>: Releases from any continuous area or volume source where the emissions are released uniformly over the area or the area represents a collection of small sources poorly quantified in terms of location (e.g., multiple vents on large manufacturing buildings, fugitive VOC sources in refineries or chemical process manufacturing plants).

Fugitive gaseous emissions resulting from collections of small sources and gaseous area source emissions of different types (e.g., process equipment, valves etc.) are modeled using techniques shown in Flowchart C-8. EPA fugitive emission factors for selected equipment are found in the EPA report Fugitive Emission Sources of Organic Compounds (Appendix A). selected air toxics, fugitive factors are also found in Appendix A (items 1 and 3). Often, areas of fugitive emissions can be specified for elevated releases such as manufacturing facilities where substantial numbers of hood and vent sources are found on the roof and fugitive emissions identified in mass balances are suspected from ventilation sources. In these cases, the area of release can be considered as a volume source using a characteristic height such as a building height. Dispersion calculations for continuous area and volume source releases are outlined in Flowcharts D-4 and D-5, respectively, with relevant calculations referenced by report section for each procedure. Receptor concentrations are estimated after determining horizontal virtual distances and corresponding dispersion parameters.

4.8 Continuous Gaseous Emissions from Land Treatment

Similar Releases: Landfarms; application of a volatile material to soil.

Land treatment emissions are modeled using the techniques outlined in release Flowchart C-9. The emissions equation is a simplification of the Thibodeaux-Hwang Emission Model, assuming ground-level application of the waste, more rapid diffusion through the oil layer, and vapor-liquid equilibrium between the oil layer and pore spaces.

• Input:

D - diffusivity of organic component in air (cm²/s)

A - land treatment surface area (cm²)

 h_{D} - depth of soil penetration by waste sludge (tilling depth)

(cm)

t - elapsed time since waste application (s)

P - vapor pressure of the constituent (atm)

MWoil - average molecular weight of the sludge (g/g-mole)

M - total oil application rate (g/cm²)

ppm - grams of organic component per million grams of waste oil

(g/10⁶g)

R - gas constant (82.06 cm³ atm/g-mole • K)

T - gas temperature (K)

• Limitations/Assumptions:

- Waste is a sludge consisting of organics in oil.
- Methods are a simplification of the Thibodeaux-Hwang Emission Model (Thibodeaux and Hwang, 1982).
- Assumes no subsurface injection, slower diffusion of organic component through air-filled pore spaces than through the oil layer, and vapor-liquid equilibrium between the air in the pore spaces and the oil layer.
- Assumes that Raoult's Law applies.
- Effective diffusivity can be assumed to be 40% of pure component diffusivity.

• Procedure:

Determine the average emission rate over the entire area, E, in q/s:

$$E = \left(\frac{DP \ MW_{oil} \ M}{5 \ h_p RT \ t}\right)^{0.5} \cdot ppm \cdot A \cdot 2 \times 10^{-6}$$

• Output:

- Emission rate, E (g/s) from a land treatment site
- Land treatment area for use in determining virtual distances for dispersion

Dispersion of land treatment emissions is simulated as an area source (Flowchart D-4).

4.9 Continuous Emissions from Municipal Solid Waste Landfills

Gaseous emissions from municipal solid waste landfills may be greater than those from properly maintained, capped hazardous waste landfills. this section presents how gaseous emissions from municipal solid waste landfills may be estimated. This information is from the draft background document for proposal of air regulations for municipal solid waste landfills (EPA, 1988a). This document explains how emissions can be estimated using either (1) an emission factor based on the amount of refuse in a landfill or (2) sampling data (e.g., field measurements of the gas flow rate and composition). The emission factor is based on measuring the amount of VOC per ton of landfilled waste using data provided by California's South Coast Air Quality Management District. The total VOC emissions determined by this procedure can be speciated using a profile from the Air Emission Species Manual, Volume I, Volatile Organic Compound Species Profiles (Appendix A, item 4). There are a number of factors contributing to the variability in from municipal solid waste landfills (e.g., waste gaseous emissions composition, landfill moisture content, age of refuse, pH and alkalinity of landfill, amount of buried waste, climate, and physical and operating characteristics of landfill). The greatest sources of uncertainty are the type and amount of waste buried in a landfill. Use of sampling data is strongly recommended (as described in the EPA background document for draft proposed regulations for municipal solid waste landfills). However, the use of an emission factor is considered appropriate as a simple screening tool, and this approach is described below, as outlined in Flowchart C-10.

• Input

- M ~ amount of refuse in place in a landfill (millions of tons)
 - either the average annual precipitation at the landfill site or the state in which the landfill is located

• Limitations/Assumptions:

- Applicable to municipal solid waste landfills.
- Provides an average VOC emission rate. (To obtain the amount of individual toxic constituents, the concentration of the individual toxic constituents is needed. The background document for the proposed regulations provides the range in concentration of toxic constituents that has been measured from landfills nationwide.)
- Emission rates are assumed to be steady-state, with no seasonal or diurnal variation. However, the effect of precipitation on emission rate is accounted for using an empirical correlation based on measured data for 20 landfills. (Refer to background document for draft proposed regulations for further information.)

• Procedure

1) If the landfill site averages less than 23 inches of precipitation per year (or, in the absence of local data, if the landfill is located in the States of AZ, CA, CO, HA, ID, MT, NV, NM, ND, SD, UT, or WY), then use the following equation to determine the emission rate, E (g/sec):

E = (0.4 g/s/million tons) M

2) If the landfill site averages 23 inches or more of precipitation per year (or, in the absence of local data, if the landfill is not in one of the states noted above), then use the following equation to determine the emission rate, E (g/sec):

E = (1.0 g/s/million tons) M

• Output

E = Average VOC emission rate (g/s)

Dispersion of emissions from a landfill is simulated as an area source (Flowchart D-4), involving determination of dispersion parameters based on virtual distances before concentrations can be calculated at each receptor location.

4.10 Continuous Emissions of Pesticides and Herbicides

Emissions resulting from the volatilization of applied pesticides or herbicides are modeled using area source techniques. Generally, screening level methods are not available for release estimates; therefore, emission rates must be user-specified as indicated in emission Flowchart C-11. The best sources of information are technical literature searches and contacts with agricultural research stations. Area source dispersion techniques, as outlined in Flowchart D-4, are used. These involve determining virtual source distances, dispersion parameters, and estimated concentrations at each receptor location.

4.11 Instantaneous Emissions Due to Equipment Openings

<u>Similar Releases</u>: Any puff or burst type release with short duration emissions resulting from the opening of equipment after processing (e.g., coke ovens or chemical reactors), from routine sampling of product during processing or gaseous emissions from disconnected lines.

Sources of this type are modeled as instantaneous point or volume sources of gaseous emissions due to the momentum of their release. Emissions can either be estimated on a source-specific basis by the user or calculated from representative emission factors, as shown in Flowchart C-12. Emissions estimates are available in AP-42 for some batch operations. VOC profiles are also available to identify toxic components (Appendix A, item 4). Simple estimates of emissions from failed or disconnected transfer lines or similar sources can be calculated from the gas volume between the break point and nearest shutoff valve.

Receptor concentrations are calculated as outlined in Flowchart D-6. A density check determines whether the cloud is negatively buoyant or passive. If passive, dispersion is simulated as a volume source with initial dimensions dependent on the circumstances of release. If volume dimensions are not known, conservative concentration estimates can be obtained by assuming a point source release.

If the cloud is negatively buoyant, dense gas concentrations are calculated. Screening techniques are available for simulating only spreading and dispersion from a low momentum, ground-level release. Descent of elevated heavy gas clouds and high momentum associated with many instantaneous releases tend to provide significant initial dilution. This dilution acts to reduce concentrations and density. A conservative screening estimate for the effects

of heavy gas, instantaneous releases can be performed assuming that the releases are undiluted (i.e., point sources) and at ground level as indicated in Flowchart D-6.

4.12 Evaporation from Quiescent or Aerated Surface Impoundments

Similar Releases: Waste lagoons and other impoundments with emissions resulting from the evaporation of volatile chemicals from liquid mixtures.

Emission rates from well-mixed aqueous waste in surface impoundments are modeled using techniques outlined in Flowchart C-13. Branching occurs to provide techniques for both quiescent and aerated impoundments. Emission estimates account for volatilization solely, with other removal mechanisms assumed to be negligible. Inputs, assumptions, and calculation procedures for emission estimates are summarized below.

• Input:

- initial concentration of the chemical in the waste (g/m³)

chemical solubility in water (g-mole/m³)

- pure component vapor pressure (atm)

- Henry's Law Constant (atm-m³/g-mole)

- area of impoundment (m²) A

F - fetch (linear distance across the impoundment) (m)

- depth of waste in impoundment (m) D

- volumetric flow rate of the waste (m³/s) Q

- time after disposal (for impoundments with no outlet flow)

POWR - aerator power (horsepower x number of aerators)
f - fraction of impoundment aerated

- number of aerators Ni

• Limitations/Assumptions:

- Equations are simplifications of methods in EPA, 1987a for quiescent surface impoundments with and without flow and for aeration basins.
- Simplified by assuming a wind speed of 5 m/s, constituent diffusivity in water of 10^{-5} cm²/s, and constituent diffusivity in air of $0.10 \text{ cm}^2/\text{s}$.
- Assumes waste is well mixed in impoundment.
- Assumes removal entirely by volatilization, with no loss due to biodegradation, seepage, or adsorption.
- Assumes waste is aqueous, with no separate organic phase.

- Reference:
 - EPA (1987a)
- Procedure:
 - 1) Calculate the equilibrium constant, K_{eq} , using

$$K_{eq} = 40.9H$$

If H is not available, then it can be approximated as:

$$H = V_p$$

2) Determine the gas-phase mass transfer coefficient, $\mathbf{k}_{g},$ in m/s using

$$k_q = 1.26 \times 10^{-2} A^{-0.055}$$

- 3) Calculate the liquid phase mass transfer coefficient, k_1 , in m/s using the appropriate equation
 - i) if F/D < 14.0

$$k_1 = 2.92 \times 10^{-6}$$

ii) if $14.0 \le F/D \le 51.2$

$$k_1 = 6.84 \times 10^{-8} \text{ (F/D)} + 3.35 \times 10^{-6}$$

iii) if F/D > 51.2

$$k_1 = 6.85 \times 10^{-6}$$

4) Determine the overall mass transfer coefficient, Kq, in m/s using:

$$K_{q} = \left(\frac{1}{k_{1}} + \frac{1}{k_{g} K_{eq}}\right)^{-1}$$

5) Determine the equilibrium or bulk concentration in the impoundment, $C_{\rm L}$, in g/m 3 using

$$C_{L} = \frac{Q C_{O}}{K_{Q} A + Q}$$

For aerated impoundments, skip to step 7.

6) Calculate the source emission rate, E, from the impoundment (g/s)

$$E = K_q C_L A$$

For disposal impoundments with no outlet flow, use the same steps 1 through 4 above and the following equation:

$$E = \frac{AD C_0}{t} \left[1 - \exp \left(-K_q t/D\right) \right]$$

7) Steps 7 through 11 are for aerated impoundments only. For the aerated impoundment calculate the turbulent liquid-phase mass transfer coefficient, kla:

$$k_{1a} = 0.2623 \text{ (POWR / A f)}$$

8) Calculate the turbulent gas-phase mass transfer coefficient, $k_{\mbox{\scriptsize ga}}$:

$$k_{ga} = 0.021 (POWR / N_i)^{0.4}$$

9) Calculate the overall turbulent mass transfer coefficient, K_{t} :

$$K_t = \left(\begin{array}{cc} 1 & + & 1 \\ \hline k_{1a} & + & \overline{K_{eq} k_{ga}} \end{array}\right)^{-1}$$

10) Determine the mass transfer coefficient resulting from the quiescent and turbulent components:

$$K = K_t f + (1-f) K_q$$

11) Emissions are obtained by calculating:

$$E = K C_{T} A$$

- Output
 - source emission rate, E, from the impoundment (g/s)
 - area of impoundment, A (m^2) , for use in virtual distance calculations

Dispersion from a surface impoundment is simulated as a continuous area source with initial dimensions equal to those of the impoundment (see

Flowchart D-4). Virtual distances are used to determine dispersion parameters which are input to the continuous point source dispersion equation to determine receptor concentrations.

4.13 Continuous Relief Valve Discharges (Two-Phase Flow)

<u>Similar Releases</u>: High pressure superheated liquid releases, continuous two-phase releases, two-phase releases from stacks.

A pressure relief event is considered to be the venting of process equipment (i.e., reactor vessels, columns, storage tanks) through rupture disks, safety relief valves, manual, or emergency vents. An event may consist of one pressure relief device discharge or a series of pressure relief device discharges stemming from the same set of circumstances. Pressure relief emissions can be either liquids or gases or some combination of the two. Other two-phase releases can result from tank leaks (see Section 4.18). Pure vapor continuous discharges are simulated using techniques in Section 4.5. Parameters for relief valve discharges are specified from plant designs. Steps in calculating two-phase releases are as follows (Flowchart C-14):

1) Calculate the fraction of liquid flash vaporized:

• Applicability:

Calculation of the fraction of liquid flash vaporized in the depressurization of a pressurized liquefied gas.

• Inputs

T_S - storage or line temperature of liquid (deg. K)

 $T_{\rm b}$ - boiling temperature at ambient pressure (deg. K)

c_D - specific heat at constant pressure (erg/(g deg. K))

L - latent heat of vaporization (erg/g)

• Limitations/Assumptions:

- The method does not allow for aerosol "rain-out".

- References:
 - World Bank (1985)
 - Wallis (1969)
- Procedure:

The fraction of liquid flashed to vapor is given by:

$$F = c_p \frac{(T_s - T_b)}{L}$$

• Output:

Fraction of a release which is vaporized to be used in calculations of cloud density

- 2) Calculate the mean density of the mixture:
 - Applicability:

Cloud density of a release containing a liquid aerosol.

• Input:

 ρ_1 - liquid density (g/cm³)

 ρ_{v} - vapor density (g/cm³)

F - mass fraction of vapor

- Limitations/Assumptions:
 - The method assumes suspension of liquid droplets.
- Reference:
 - Wallis (1969)
- Procedure:

Calculate the mean mixture density by:

$$\rho_{m} = \frac{1}{(F/\rho_{v}) + (1-F)/\rho_{I}}$$

- Output:
 - Density of a vapor/liquid aerosol cloud (g/cm³)
- 3) Calculate the two-phase outflow:
 - Applicability:

Two-phase (vapor/liquid aerosol) release rates resulting from major leaks in the vapor space of a containment for a pressurized superheated liquid.

• Inputs:

A - Release area (cm^2)

 ρ_{m} - mixture density (g/cm³) ρ_{1} - line or storage pressure (dynes/cm²)

- Limitations/Assumptions:
 - Assumes homogeneous flow with components in equilibrium.
 - Pressure is assumed to drop to atmospheric pressure immediately on release. This is conservative for higher pressure releases.
 - C_d, the coefficient of discharge, is assumed to be 0.8.
- References:
 - World Bank (1985)
 - Hunsaker and Rightmire (1947)
- Procedure:

Calculate the discharge rate: (g/s)

$$q_m = 0.76 \text{ A } \sqrt{\rho_m P_1}$$

• Output:

Total discharge rate, q_m , in g/s for the liquid/vapor mixture

Screening estimates can be obtained using Flowchart D-1 assuming that the density used is that of the mixture. The mass emission rate is equivalent to the total release rate from the valve or tank. Density checks are performed to determine whether the resultant plumes may be affected by gravitational spreading. The dispersion of the resultant cloud assumes no change of state from the initial value. Continuous two-phase release events are some of the most frequent scenarios in which dense gas effects may be indicated. Estimates of plume density will determine if these effects are important. If the plume is dense, worst case estimates are made using the RVD model for which a range of wind speeds should be input. If the plume is not dense, point source techniques are used to simulate dispersion (Flowchart D-2). If the plume is in the cavity, different procedures may be necessary depending on receptor location. If the plume is not in the cavity or wake, normal point source techniques apply.

Initial dilution of high pressure releases should be considered, but techniques are not currently available. In addition, neither fallout nor the evaporation of droplets is not included.

4.14 Instantaneous Relief Valve Discharges (Two-Phase)

<u>Similar Releases</u>: This class represents any instantaneous two-phase pressure relief event from relief valves or pressurized tank lines or vessels.

Relief valve or rupture disk discharges and other two-phased releases are generally site specific and emissions must be specified as indicated in Flowchart C-15. Atmospheric dispersion screening estimates are made using instantaneous dispersion modeling techniques.

Dispersion modeling follows a determination of whether the cloud is affected by negatively buoyant forces as shown in Flowchart D-6. The density determination is made based on the mean cloud density (see equation in Section 4.13), and subsequent simulations of dispersion are based on the total cloud mass. If the puff is not dense, instantaneous point source techniques apply.

4.15 Low Volatility Liquid Leaks from Pipes

<u>Similar Releases</u>: Continuous low volatility liquid leaks from connectors, flanges, transfer lines or pumps; finite liquid releases from disconnected transfer lines.

Liquid releases can occur in the form of finite spills or continuous leaks. For these screening calculations, it is assumed that finite spills are small and will form a pool with a 1 cm depth. A steady-state evaporation rate is estimated and is conservatively assumed to persist throughout the dispersion averaging period. For continuous releases, Flowchart C-16 indicates that if liquid leak rates are unknown, the leak rate equals the maximum flow rate in the pipe. The released liquid is then assumed to pool in an area which is the lesser of the unbounded pool spread area, impoundment boundary or the area over which the liquid spreads before reaching the impoundment boundary (i.e., pools not contained in the impoundment). Finally, the steady state emission rate is calculated. Equations for these calculations are provided below.

• Input:

MW - molecular weight (g/g-mole)

 A_C - area for confined releases (m²)

 $\mathbf{T}_{\mathbf{p}}^{-}$ - pool surface temperature (deg. K) assumed equal to ambient

temperature

u - wind speed (m/s)

q1 - liquid release rate (g/s)

 P^- - vapor pressure (dynes/cm 2) at surface temperature $T_{
m p}$

V - finite liquid release volume (m³)

• Limitations/Assumptions:

- The model is steady state and applicable to single phase releases.
- Phase change of superheated liquids is not considered.
- Evaporation begins after pool formation.

- Minimum pool depth is 1 cm.
- Pool spreading reaches a steady-state when the liquid release rate equals the evaporation rate.
- References:
 - NOAA (1988)
- Procedure:
 - 1) Calculate the intermediate parameter B consolidating terms of the model:

$$B = 1.54 \times 10^{-4} \frac{u^{0.78 \text{ MW}}0.67 \text{ p}}{T_p}$$

- 2) Estimate liquid release amount or rate. For finite releases use a known volume or estimate the released volume as the volume of the disconnected or failed transfer line. For continuous liquid leaks, assume that the liquid release rate, q_1 , is equal to the mass flow rate in the pipe or line.
- 3) Calculate the area of the pool. For finite releases:

$$A = 100 V$$

where: $V = \text{liquid release volume } (m^3)$ Proceed to step 4.

For continuous releases, the area of the evaporating pool is calculated as the smaller of the impoundment area or the area at which evaporation across the pool equals flow into the pool.

$$A = \min. \begin{cases} A_{c} \\ \left(\frac{q_{1}}{B}\right)^{1.06} \end{cases}$$

4) The steady state emission rate q_v (g/s) is given by:

$$q_v = BA 0.94$$

- Output:
 - Steady state emission rate (g/s)
 - Pool area (m²)

Dispersion from the pooled liquid is simulated using continuous area source techniques (Flowchart D-4). Low volatility liquids are expected to pool in a ground level area source from which emissions are generated by evaporation. Pool dimensions are used to determine virtual distances and dispersion parameters for area source modeling of passive releases.

4.16 Low Volatility Liquid Leaks from Tanks

Similar Releases: Low volatility liquid leaks from containment or reactor vessels (i.e., leak below the liquid level).

As indicated in release Flowchart C-17, liquid release rates from a tank are computed and used as input to the evaporation model, where pool spread area and a steady state emission rate are estimated. Equations for the calculation are given below.

1) Calculate Liquid Release Rate

• Input:

 ρ_1 - liquid density (g/cm³)

A - hole or puncture area (cm²)

P_a - atmospheric pressure (dynes/cm²)

Pt - tank pressure (dynes/cm²)

H - height of the liquid column above the hole (cm)

Cd - coefficient of discharge

• Limitations/Assumptions:

- Does not simulate time dependent release rates for tanks with decreasing pressure.
- The coefficient of discharge varies between 0.6 and 1.0 as a function of release geometry and Reynolds number. For screening purposes, assume $C_{\rm d}=0.8$.

• References:

- Environmental Protection Service (1985)
- Hunsaker and Rightmire (1947)

• Procedure:

Calculate the liquid flow rate by:

Flow rate (g/s)

$$q_1 = 0.8 \text{ A } \rho_1 \sqrt{1960 \text{ H} + \frac{2 (P_t - P_a)}{\rho_1}}$$

2) Proceed to apply the Evaporation Model from Section 4.15 for continuous releases beginning in step 1 using the value for q_1 derived above.

4.17 High Volatility Liquid Leaks from Pipes

Small pipe leaks of highly volatile liquids are assumed, for screening purposes, to boil off instantaneously, resulting in a plume which is simulated with a continuous point source dispersion model. Emission rate (g/s) is assumed to equal the pipe flow rate, as indicated in release Flowchart C-18.

Dispersion of the plume is simulated with a continuous point source dispersion model (Flowchart D-2). For screening estimates, it is assumed that the leak is in the cavity zone and plume rise calculations are not required. In addition, due to the small leak size, it is assumed that the release has low momentum and is passive rather than negatively buoyant (i.e., not a dense gas).

4.18 High Volatility Liquid Leaks from Tanks

Small tank leaks of highly volatile liquids are simulated using an equation to calculate liquid release rates and an assumption of instant evaporation, resulting in an emission rate equal to the release rate (see release Flowchart C-19). The emission rate calculation procedures are given below. (Note, in the special case of pressurized releases from moderate leaks below the liquid level of the tanks, techniques used are those in Section 4.13.)

• Applicability:

Calculation of release rate of a liquid from a storage tank or other vessel with a small leak below the liquid level.

• Input:

 ρ_1 - liquid density (g/cm³)

- hole or puncture area (cm²)

P_a - atmospheric pressure (dynes/cm²)
P_t - tank pressure (dynes/cm²)

H - height of the liquid column above the hole (cm)

Cd - coefficient of discharge

• Limitations/Assumptions:

- Does not simulate time dependent release rates for tanks with decreasing pressure.
- The coefficient of discharge varies between 0.6 and 1.0 as a function of release geometry and Reynolds number. For screening purposes, assume $C_d = 0.8$.

• References:

- Environmental Protection Service (1985)
- Hunsaker and Rightmire (1947)

• Procedure:

Calculate the liquid flow rate by:

Flow rate (g/s)

$$q_1 = C_d \quad A \qquad \rho_1 \quad \sqrt{1960 \quad H + \frac{2 (P_t - P_a)}{\rho_1}}$$

• Output:

Liquid discharge rate in g/s for use in the dispersion model.

Dispersion of the plume is conservatively simulated with a continuous point source dispersion model (Flowchart D-2). For screening estimates, it is assumed that the leak is in the cavity zone and plume rise calculations are not required. In addition, due to the small leak size, it is assumed that the gas release has low momentum and is passive rather than dense.

5.0 ATMOSPHERIC DISPERSION ESTIMATES

This section provides screening techniques and equations to determine receptor concentrations resulting from toxic releases. Methods are provided to examine and estimate the impacts of cloud density, plume rise, initial dilution, and atmospheric dispersion on downwind concentrations. This section is designed to be used in conjunction with the dispersion flowcharts in Appendix D. Prior to using this section, the user should estimate emissions using the release scenario descriptions and emission estimating techniques of Section 4 along with the flowcharts in Appendix C. The final step of the appropriate release scenario flowchart (Appendix C) will direct the user to the first step of the appropriate dispersion flowchart and subsection below.

Dispersion estimates for continuous and instantaneous emissions are provided by the techniques described in this section. Averaging times represented in the estimates are determined by the dispersion parameters used. It is assumed that continuous estimates will result in hourly average concentrations and that instantaneous estimates represent peak concentrations averaged over periods of less than a minute. The user is directed to Appendix E if approximations to other averaging periods are required.

5.1 Cloud Densities

- 5.1.1 Calculations to Determine the Relative Density of Instantaneous Releases
- Applicability:

All instantaneous releases

• Input

 $\rho_{\rm v}$ - density of the gas or vapor (g/cm³)

 m_n - mass of each constituent (g)

 M_n - molecular weight of each constituent (g/g-mole)

u - wind speed (m/s)

 T_S - temperature of the material released (deg. K)

Ta - ambient temperature (deg. K)

 M_S - molecular weight of material released (g/g-mole)

 V_{i} - volume released (m³) (calculated using density and release

amount)

 ρ_a - density of air (g/cm³)

- Limitations/Assumptions:
 - It is assumed that neutrally and positively buoyant releases will be simulated with passive dispersion models.
 - Releases which are negatively buoyant may disperse as passive materials if atmospheric turbulent energy exceeds or dominates buoyancy effects.
- References:
 - Havens and Spicer (1985)
 - Briggs (Randerson, 1984)
- Procedure:
 - Density calculations begin with an estimate of molecular weight for gas mixtures

$$M_{S} = \frac{\sum m_{n}}{\sum (m_{n}/M_{n})}$$

2) If:

$$\frac{T_s}{M_s} \rightarrow \frac{T_a}{28.9}$$

dispersion is not affected by negative buoyancy effects and passive techniques can be used.

3) If the release Richardson number

Ri = 2,722
$$\left(\frac{M_s T_a}{28.9 T_s} - 1\right) \frac{V_i^{1/3}}{u^2} \ge 30$$

then effects of the negative buoyancy should be considered. Otherwise passive techniques can be used. Note that the following density ratios may be substituted, for the parenthetical expression above:

$$\left(\frac{\rho_{v} - \rho_{a}}{\rho_{a}}\right)$$
 or $\left(\frac{\rho_{v}}{\rho_{a}}\right)$

5.1.2 Calculations to Determine the Relative Density of Continuous Releases

• Applicability:

All continuous releases

• Input:

mn - mass of each constituent (g)

 M_n - molecular weight of each constituent (g/g-mole)

wind speed (m/s)

 T_s - temperature of the material released (deg. K)

Ta - ambient temperature (deg. K) d - effective diameter (m)

- volume emission rate (m³/s) specified or calculated from

mass release rate and density

Mg - molecular weight of material released (g/g-mole)

• Limitations/Assumptions:

- It is assumed that neutrally and positively buoyant releases will be simulated with passive dispersion models.
- Releases which are negatively buoyant may disperse as passive materials if they are small enough such that atmospheric turbulent energy exceeds or dominates buoyancy effects.

• References:

- Havens and Spicer (1985)
- Briggs (Randerson, 1984)

• Procedures:

 Density calculations begin with an estimate of molecular weight for gas mixtures

$$M_{s} = \frac{\sum m_{n}}{\sum (m_{n}/M_{n})}$$

2) If:

$$\frac{T_s}{M_s} \rightarrow \frac{T_a}{28.9}$$

dispersion is not affected by negative buoyancy effects and plume rise and passive modeling procedures should be applied. Otherwise, proceed to Step 3.

'3) The release Richardson number is calculated:

$$Ri = 2.722 \left(\frac{M_s T_a}{28.9 T_s} - 1 \right) \frac{V}{u^3 d}$$

where V is the volume release rate which is either specified or calculated from the mass release rate. The volume rate is obtained by multiplying the mass release rate by the molar volume at the release temperature and dividing by the molecular weight.

$$V = \frac{q_V MV}{M_c}$$

where MV is the molar volume (m³/mole) and $q_{\rm V}$ is the mass release rate (g/s). Alternatively, if the vapor (gas) density is known, the volume rate is the mass rate divided by the density.

The diameter, d, in the equation is a scale length or effective diameter. For gaseous releases, it is taken to be stack or vent diameter. For high volatility liquid releases, it is taken to be the diameter of a circular plane situated perpendicular to the direction of material transport by the wind away from the leak or

$$d = \sqrt{\frac{4 \text{ V}}{--}}$$

The parenthetical terms in the Richardson number equation can be replaced by the density ratios

$$\left(\frac{\rho_{v} - \rho_{a}}{\rho_{a}}\right)$$
 or $\left(\frac{\rho_{v}}{\rho_{a}} - 1\right)$

if densities of the vapor (gas) and air are known.

If Ri \geq 30, the effects of the negative buoyancy should be considered. Otherwise, plume rise and passive modeling procedures should be applied.

5.2 Plume Rise Calculations

5.2.1 Mean Molecular Weight for Mixtures of Gases

• Applicability:

Plume rise must be calculated for a complete effluent stream. This calculation provides a mean molecular weight to be used in determining buoyancy flux.

• Input:

 m_n - mass of each constituent (g)

 M_n - molecular weight of each constituent (g/g-mole)

• Procedure:

Compute the mean molecular weight in (g/g-mole) by the following

$$M_{s} = \frac{\sum m_{n}}{\sum (m_{n}/M_{n})}$$

5.2.2 Flare Plume Rise

Applicability:

Continuous flares

• Input:

V - volume release rate from the flare (m^3/s)

 ${\bf f_i}$ - volume fraction of each component of the flare gas ${\bf h_S}$ - stack height (m)

H_i - net heating value of each component (cal/g-mole)

• Limitations/Assumptions:

- Plume rise for continuous flares must be calculated using special techniques to account for radiational heat losses and flame bending in the wind.
- 55 percent of the total heat output of the flare is radiated and unavailable for plume rise.
- The flare flame is assumed to be tilted 45 degrees from vertical.

- Source height for the flare consists of the physical stack height and the height from flare outlet to flame tip.

• References:

- Beychok (1979)
- Leahey and Davies (1984)

• Procedures:

The EPA regulates the design of flares used as control devices in 40 CFR 60.18. In the regulation, minimum values of net heating value for the combusted gas and exit velocity for flares, and air and steam assisted flares are specified. It should be confirmed prior to calculating flare plume rise that the flare is permitted under this regulation.

1) Calculate the total heat release rate from the flare gas combustion by:

$$Q_t$$
 (cal/s) = 44.64 V $\sum_{i=1}^n f_i H_i$

where the summation is over the n components of the flare gas stream, f_i is the volume fraction, and H_i is the net heating value of each component.

2) Calculate the vertical flame tip height, hf (meters)

$$h_f = 4.56 \times 10^{-3} Q_t^{0.478}$$

and the effective release height before plume rise (meters) as

$$h_{se} = h_{s} + h_{f}$$

3) Calculate buoyancy flux (m^4/s^3) based on the heat release rate:

$$F = 1.66 \times 10^{-5} Q_{+}$$

- Output
 - h_{se}, flare flame tip height (m)
 - F, buoyancy flux (m^4/s^3)

5.2.3 Buoyancy Plume Rise

• Applicability:

Plume rise for continuous sources with buoyant releases

• Input:

 m_n - mass of each constituent (g)

 M_n - molecular weight of each constituent (g/g-mole)

F - buoyancy flux (m⁴/s³) x - downwind distance (m)

h_s - stack height (m)

Ta - ambient temperature (K)

u - wind speed (m/s)

T_S - stack gas temperature (K)

M_S - mean molecular weight of effluent (g/g-mole)

V_S - stack exit velocity (m/s) d - diameter of stack (m)

• Reference

- Briggs (Randerson, 1984)

• Procedures

1) If calculating plume rise for a flare, use the flux determined in Section 5.2.2 and start with Step 3. For other sources, compute the mean molecular weight by:

$$M_{s} = \frac{\sum m_{n}}{\sum \frac{m_{n}}{M_{n}}}$$

2) If calculating plume rise from a flare, use the flux determined in Section 5.2.2 and start with Step 3. For other sources, calculate the buoyancy flux, $F(m^4/s^3)$, using either a mixture or single component molecular weight and the following:

$$F = 2.45 \text{ V}_{s}d^{2} \left(\frac{(T_{s}/M_{s}) - (T_{a}/28.9)}{(T_{s}/M_{s})} \right)$$

If F is negative (or zero), the plume is assumed to be passive and release height, h_s , should be used as the effective plume height, H, in dispersion calculations (i.e., $\Delta h = 0$ and continue with Step 6).

If F is positive, the plume is buoyant and plume rise can be calculated with the procedures that follow.

3) Determine the distance to final plume rise (meters):

neutral and unstable conditions:

$$\mathbf{x_f} = \begin{cases} 49 & \text{F}^{0.625} & \text{for } \text{F } < 55 \text{ m}^4/\text{s}^3 \\ 119 & \text{F}^{0.4} & \text{for } \text{F } \geq 55 \text{ m}^4/\text{s}^3 \end{cases}$$

stable conditions:

$$x_f = 2.0715 \text{ u s}^{-0.5}$$

where

$$s = \frac{9.81 \frac{\Delta \Theta}{\Delta z}}{T_a}$$

and $\frac{\Delta \Theta}{-}$ equals 0.02 K/m and 0.035 K/m for E and F stability, Δz

respectively.

4) If the receptor distance, x, is less than x_f , calculate plume rise (meters) for neutral and unstable conditions as:

$$\Delta h = 1.6 \frac{F^{0.33} x^{0.667}}{u}$$

For $x \ge x_f$, substitute $x = x_f$ in the above equation.

5) Estimate the effective plume height (meters) as

$$H = h_S + \Delta h$$

For flares, the stack height h_s is defined as h_{se} .

5.3 Dispersion Parameters

5.3.1 <u>Horizontal and Vertical Dispersion Parameters for Continuous</u> Emission Releases

• Applicability:

Parameters estimating the horizontal and vertical dispersion of a plume for use in Gaussian dispersion models.

• Input:

- x downwind distance (m) for point and area sources
- xy horizontal virtual distance plus receptor distance (m), for use with area and volume sources
- $\mathbf{x_Z}$ vertical virtual distance plus receptor distance (m), for use with volume sources
- A-F stability class

• Limitations/Assumptions:

- The parameters were developed from data collected over 10 min. periods but have been used extensively to provide concentration estimates for one hour averaging periods

• Reference:

- Turner (1970)

• Procedure:

- 1) Figures 5-1 and 5-2 provide estimates of dispersion parameters versus downwind distance (i.e., source-receptor distance) for each stability class. Note that downwind distance in the figures is given in kilometers.
- 2) Virtual point source distances for each stability class can be determined by first locating the value of the dispersion parameter for each stability class and then locating the initial distance on the x axis.
- 3) Dispersion parameters for modeling can be determined by selecting the value of the dispersion parameter for each receptor distance and stability.

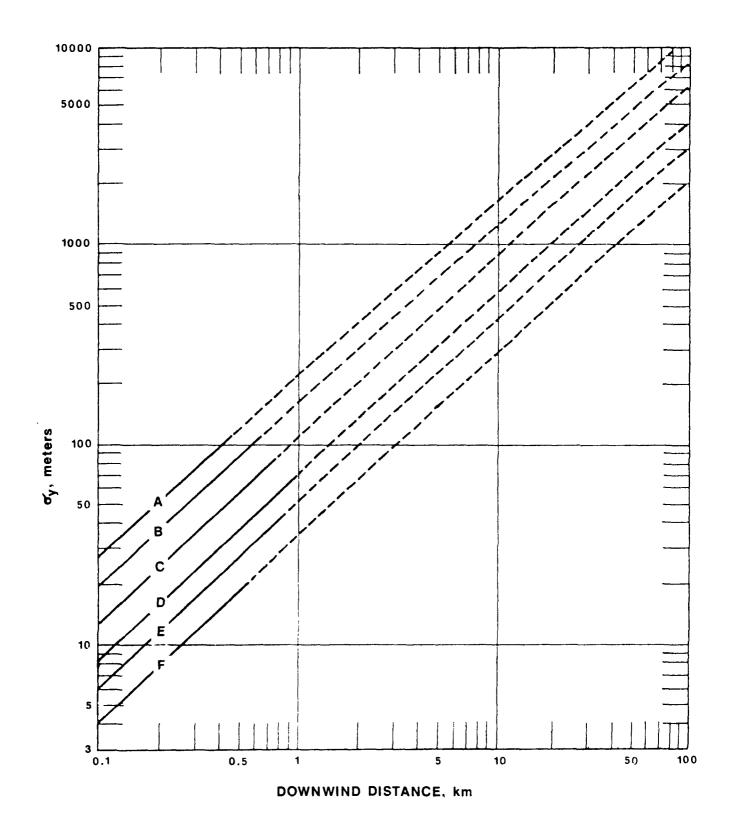


FIGURE 5-1. HORIZONTAL DISPERSION PARAMETER (σ_y) AS A FUNCTION OF DOWNWIND DISTANCE AND STABILITY CLASS (Continuous Releases; Turner, 1970)

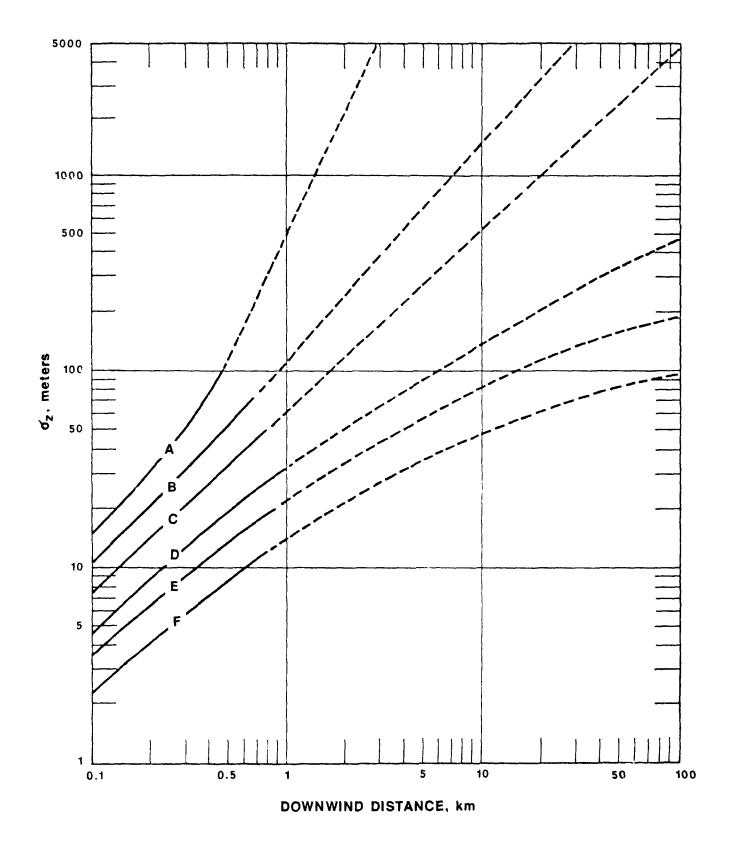


FIGURE 5-2. VERTICAL DISPERSION PARAMETER (σ_z) AS A FUNCTION OF DOWNWIND DISTANCE AND STABILITY CLASS (Continuous Releases; Turner, 1970)

• Output:

 σ_{y} , σ_{z} - horizontal and vertical continuous plume dispersion parameters for each stability class and receptor distance (m)

5.3.2 <u>Horizontal and Vertical Dispersion Parameters for Instantaneous</u> <u>Emission Releases</u>

• Input:

x - downwind distance to the receptor (m) A-F - stability class

• Limitations/Assumptions:

- Parameters are given for three stability classes. It is assumed that the unstable class includes PG classes A C, the neutral category includes PG class D, and the stable class includes PG classes E and F.
- Dispersion parameters represent instantaneous peaks of one minute duration.

• Reference:

- Petersen (1982)

• Procedure:

- 1) Figures 5-3 and 5-4 provide instantaneous dispersion parameters relative to the puff center for each stability class and downwind distance (i.e., source-receptor distance). Note that downwind distance in the figures is given in kilometers.
- 2) Horizontal dispersion parameters, represented by σ_x and σ_y , are assumed to be equal and are given by σ_r in the figures.
- 3) Dispersion parameters can be determined by selecting a value for each downwind distance and stability class.

• Output:

- Vertical, crosswind, and downwind dispersion parameters, σ_z , σ_v , and σ_x , for each downwind position of the puff (m)

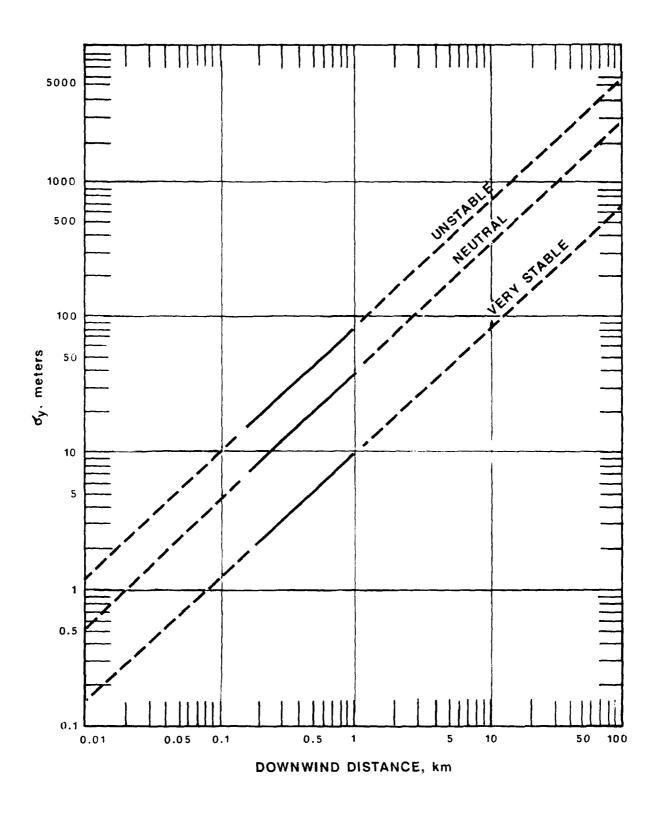


FIGURE 5-3. HORIZONTAL DISPERSION PARAMETER (δ_y) AS A FUNCTION OF DOWNWIND DISTANCE AND STABILITY CLASS (Instantaneous Releases; Petersen, 1982)

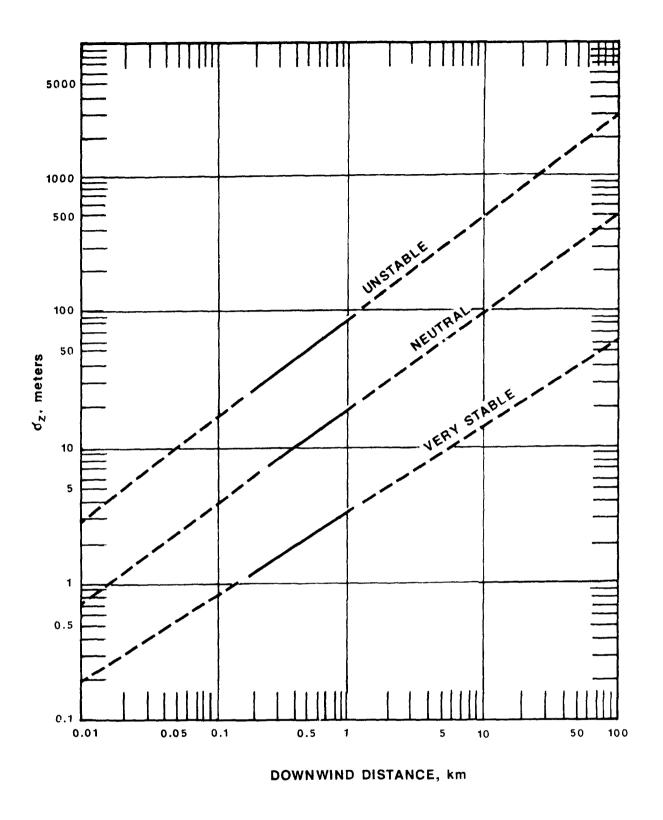


FIGURE 5-4. VERTICAL DISPERSION PARAMETER (σ_z) AS A FUNCTION OF DOWNWIND DISTANCE AND STABILITY CLASS (Instantaneous Releases; Petersen, 1982)

5.3.3 Horizontal and Vertical Dispersion Parameters for Wake Effects

Applicability:

Continuous emission point sources

• Inputs:

stack height (m) h_b - building height (m)

W - building width (m)

L - building length (m)

h_m - momentum plume rise (m) at x = 2h_b (see Section 5.6.1)

A-F - stability

• Limitations/Assumptions:

For stack to building height ratios (h_s/h_b) < 1.5, EPA recommends the use of the Schulman and Scire method in the ISC model. However, this method is not simple enough to use in this workbook. The Huber and Snyder technique is used here.

- Reference:
 - Huber and Snyder technique derived from the ISC model (EPA, 1987c)
- Procedure:
 - 1) Determine the maximum projected building width:

$$h_w = (L^2 + W^2)^{\frac{1}{2}}$$

2) Determine if the plume will be affected by the wake by comparing the plume height $(h_s + h_m)$ to the depth of the wake region:

If:

$$h_{s} + h_{m} \rightarrow \begin{cases} 2.5 h_{b} \\ 1.5 h_{w} + h_{b} \end{cases}$$
, or

Wake effects are not significant and need not be considered. Proceed to Flowchart D-3.

3) Determine if the receptor is located in the cavity region:

If:

$$x < 3 h_a$$

where:

$$h_{a} = \begin{cases} h_{b} \text{ for squat buildings } (h_{w} > h_{b}) \\ h_{w} \text{ for tall buildings } (h_{w} < h_{b}) \end{cases}$$

then the downwash concentrations cannot be estimated with screening techniques. Otherwise, proceed with the wake analysis.

4) Calculate plume dispersion parameters:

$$\sigma_{z} = \begin{cases} 0.7 h_{a} + 0.067 (x - 3h_{a}) & \text{for } 3h_{a} \le x \le 10 h_{a} \\ \sigma_{z} (x + x_{vz}) & \text{for } x \ge 10h_{a} \end{cases}$$

If:

$$h_s + h_m < 1.2 h_s$$

then

en
$$\sigma_{y} = \begin{cases} 0.35 \text{ h}_{a} + 0.067 (x - 3h_{a}) & \text{for } 3h_{a} \leq x < 10h_{a} \\ \sigma_{y} (x + x_{vy}) & \text{for } x \geq 10h_{a} \end{cases}$$

Otherwise σ_{V} is obtained from Section 5.3.1.

 $x_{\mathbf{v}\mathbf{y}}$ and $x_{\mathbf{v}\mathbf{z}}$ are the horizontal and vertical virtual distances for wake effects as calculated in Section 5.5.3.

- 5) Use dispersion parameters from 4) to calculate concentrations using Section 5.6.4.
- Output:

 $\sigma_{\rm V}$ and $\sigma_{\rm Z}$ for wake effects.

5.4 Buoyancy-Induced Initial Dilution

• Applicability:

Turbulent motion of buoyant plumes and associated entrainment of air provides initial dilution of dispersing clouds. Pasquill (1976) provides a method for computing the effect of this dilution by modifying the dispersion parameters used in continuous sources models.

• Input:

 σ_z , σ_y - Dispersion parameters used in modeling (m) from Section 5.4.1(a)

Δh - Distance dependent buoyant plume rise (m)

• Limitations/Assumptions:

- For small sources the effect may be negligible.
- For most elevated sources, neglect of this step results in a less conservative result (i.e., lower predicted concentrations).

• Procedure:

1) Calculate the modified horizontal dispersion parameter

$$\sigma_{y} = (\sigma_{y}^{2} + (\Delta h/3.5)^{2})^{1/2}$$

2) Calculate the modified vertical dispersion parameter:

$$\sigma_z = (\sigma_z^2 + (\Delta h/3.5)^2)^{1/2}$$

5.5 Virtual Source Distances

5.5.1 Virtual Distances for Area Sources

• Applicability:

Continuous or instantaneous releases of pollutants from area sources or initial clouds of pollutants which cover a significant near-source area.

• Input:

W - area source width (m)

A-F - stability class

- Limitations/Assumptions:
 - An area source can be represented by a large plume or puff with initial spreading or dispersion similar to that which would occur with a point source located at some distance upwind of the source.
 - Centerline concentrations near the area source will be very conservative.
- Reference:
 - Turner (1970)
- Procedure:
 - 1) Determine the width of the area source and estimate the initial horizontal dispersion parameter by:

$$\sigma_{yo} = W / 4.3$$

- 2) Determine the downwind distance corresponding to the initial horizontal dispersion parameter using either Figure 5-1 (for continuous releases) or 5-3 (for instantaneous releases). This distance is the virtual point source distance, $x_{\rm V}$. Convert this distance to meters.
- 3) For both instantaneous and continuous sources, dispersion can be simulated by using the distance, in meters:

$$x_v = (x_r + x_v)$$

where x_r is the distance to each receptor from the area source center. In the calculation of dispersion parameters, the distance x_v is used for determining σ_v .

4) In comparisons of the source/receptor distance relative to position of maximum concentrations, the receptor distance, x_r , should be used.

• Output:

- Virtual point source distance and total distance to be used in determining plume spreading parameters for area sources.

5.5.2 <u>Virtual Distances for Volume Sources</u>

• Applicability:

Continuous/instantaneous ground level releases of pollutants which, as a result of release characteristics or initial dispersion, can be represented as a cloud with significant volume at the start of dispersion away from a source location.

• Input:

W - cloud or source width

 H_V - cloud depth (m)

A-F - stability class

• Limitations/Assumptions:

- A pollutant cloud with initial spreading or dilution can be represented by a point source located sufficiently far upwind such that the simulated puff or plume is bounded by the initial cloud dimensions.
- Centerline concentrations within 10 side widths of the volume source will be conservative.

• Reference:

- Turner (1970)

• Procedure:

- 1) Use the techniques of Section 5.5.1 to determine a horizontal virtual source distance, x_v , for use with the volume source.
- 2) Determine the depth of the volume source and the initial vertical dispersion parameter by:

$$\sigma_{zo} = H_v / 2.15$$

- 3) From Section 5.3.1 (for continuous releases) or 5.3.2 (for instantaneous releases), determine the downwind distance corresponding to the initial vertical dispersion parameter. This distance is the vertical virtual point source distance, Xvz.
- 4) For both instantaneous and continuous sources, dispersion estimates are made by determining the vertical and horizontal parameters using the distances

$$x_v = (x_r + x_v)$$

for the horizontal parameter, and

$$x_z = (x_r + x_{vz})$$

for the vertical parameter.

• Output:

- Virtual source distances and total distances for determining plume and puff spread parameters to be used in dispersion models for volume sources.

5.5.3 Virtual Distances for Wake Effects

• Applicability:

Continuous emission point sources

• Inputs:

stack height (m) - building height (m) building width (m) L - building length (m)

 h_m - momentum plume rise (m) at x = $2h_b$ (see Section 5.6.1) u - wind speed (m/s)

A-F - stability

• Limitations/Assumptions:

For stack to building height ratios (h_s/h_b) < 1.5, EPA recommends the use of the Schulman and Scire method in the ISC model. However, this method is not simple enough to use in this workbook. The Huber and Snyder technique is used here.

- Reference:
 - Huber and Snyder technique derived from the ISC model (EPA, 1987c)
- Procedure:
 - 1) Determine the maximum projected building width:

$$h_w = (L^2 + W^2)^{1/2}$$

2) Determine if the plume will be affected by the wake by comparing the plume height $(h_s + h_m)$ to the depth of the wake region:

If:

$$h_s + h_m \rightarrow \begin{cases} 2.5 h_b \\ 1.5 h_w + h_b \end{cases}$$
, or

Wake effects are not significant and need not be considered. Proceed to Flowchart D-3.

3) Determine if the receptor is located in the far wake region:

If:

$$x > 10 h_a$$

where:
$$\mathbf{h_a} \; = \; \left\{ \begin{array}{l} \mathbf{h_b} \; \text{for squat buildings (h_w > h_b)} \\ \\ \mathbf{h_w} \; \text{for tall buildings (h_w < h_b)} \end{array} \right.$$

then proceed with step 4. Otherwise, wake effects virtual distances are not needed (proceed with near wake calculations in Section 5.3.3).

4) Calculate the horizontal and vertical plume dispersion parameters at $x = 10h_a$:

$$\sigma_v = 0.82 h_a$$

$$\sigma_z = 1.2 h_a$$

:
$$h_{a} = \begin{cases} h_{b} \text{ for squat buildings } (h_{w} > h_{b}) \\ h_{w} \text{ for tall buildings } (h_{w} < h_{b}) \end{cases}$$

- 5) Determine the downwind distance corresponding to the enhanced horizontal dispersion parameter using either Figure 5-1 (continuous releases) or 5-3 (instantaneous). Similarly, use Figures 5-2 or 5-4 to determine the distance corresponding to the enhanced vertical dispersion parameters for the stability category of interest.
- 6) Use the horizontal virtual distance, x_{vy} , and the vertical virtual distance, x_{vz} , when calculating wake effects dispersion parameters for the far wake using Section 5.3.3.

• Output:

- $x_{\mathbf{v}\mathbf{y}}$ and $x_{\mathbf{v}\mathbf{z}}$ for wake effects

5.6 Concentration Calculations

5.6.1 Cavity Modeling

• Applicability:

Concentrations from continuous point sources trapped within the recirculation zone in the lee of a building.

• Input:

hb - height of building (m)

Lb - lesser dimension (height or projected width of building)(m)

Ta - ambient air temperature (K) Ts - stack exit temperature (K)

v_s - stack exit velocity (m/s)

d - stack diameter (m)
u_C - critical wind speed (m/s)

hs - stack height (m)

- crosswind building dimension (m)

A - cross-sectional area of building normal to wind (m^2)

u - wind speed (m/s)

L - alongwind building dimension (m)

• Limitations/Assumptions:

- The model simulates cavity concentrations with a uniform distribution.

• Reference:

- EPA, 1984 (Regional Workshop on Air Quality Modeling: A Summary Report)

• Procedure:

1) Compare the stack height to the cavity height. Calculate the cavity height h_c (m):

$$h_C = h_b + 0.5(L_b),$$

If the stack height is greater than or equal to the cavity height, no further cavity analysis is required. Proceed to perform the wake effects analysis (Section 5.5.3). If the stack height is less than the cavity height, proceed to Step 2.

2) Estimate the momentum plume rise for neutral atmospheric conditions. First compute the momentum flux, F_m (m^4/s^2):

$$F_m = (T_a/T_s) v_s^2 d^2/4$$

3) Next, compute the momentum plume rise h_m (m):

$$h_{\rm m} = \left(\frac{3F_{\rm m} \cdot x}{b^2 u_{\rm c}^2}\right)^{1/3}$$

where: $b = (1/3 + u_c/v_s)$.

x = downwind distance (m). Use $x = 2h_b$.

Assume a critical wind speed $u_c = 10 \text{ m/s}$

4) Compute the plume height, H_D (m):

$$H_D = h_S + h_M$$

If the plume height is greater than or equal to the cavity height calculated in Step 1, then no further cavity analysis is required. Proceed to the wake effects analysis (Section 5.5.3). If the plume height is less than the cavity height, proceed to Step 5.

5) Estimate the downwind extent of the cavity. Compute the cavity length (x_r) , measured from the lee side of the building (m):

For short buildings (L/hb<2):

$$x_r = \frac{(a)(W)}{1.0 + b(W/h_b)},$$
where: $a = -2.0 + 3.$

where: $a = -2.0 + 3.7 (L/h_b)^{-0.33}$ and

$$b = -0.15 + (0.305) (L/h_b)^{-0.33}$$

For long buildings (L/h_b \geq 2):

$$x_r = \frac{1.75(W)}{1.0 + 0.25(W/h_b)},$$

Next, compare the cavity length to the closest distance to the plant property line. Consider only plant property to which public access is precluded. If the cavity does not exceed this distance, then it may be assumed that cavity effects will not impact ambient air, and no further cavity analysis is required. Proceed to the wake effects analysis. If the cavity extends beyond plant property, proceed to step 6.

6) Estimate impacts within the cavity. "Worst case" concentration impacts (C) can be estimated by the following approximation (g/m^3) :

$$C = \frac{Q}{1.5(A)(u)},$$

where:

Q = emission rate (q/s),

A = cross-sectional area of building normal to wind (m^2) equals W x h_b and

u = wind speed (m/s).

For u, choose the lowest wind speed likely to result in entrainment of most pollutants into the cavity. If no data are available from which the minimum speed can be estimated, assume a worst case wind speed of 1 m/s.

Since both the cavity concentration and cavity length calculations depend on building orientation relative to the wind, it is advisable to repeat the calculations using two orientations of the building; one with the minimum dimension alongwind and the other with maximum dimension alongwind and choosing the highest concentration.

5.6.2 Heavy Gas Model - Instantaneous Releases

• Applicability:

The model described is applicable to instantaneous ground level releases of dense gases in flat terrain. The model neglects evaporation of condensation of drops and vapors in clouds, heat and mass exchange with underlying surface, radiation flux and chemical reactions.

• Inputs:

R_O - initial cloud radius (m)

u - wind speed (m/s)

 V_{o} - initial cloud volume (m³) ρ_{a} - density of air (g/m³) ρ_{g} - density of gas (g/m³) κ_{r} - downwind receptor distance (m)

• Limitations/Assumptions:

Gases which are heavier than air disperse under the influence of buoyant and turbulent forces. Models for simple cases of gases much heavier than air on flat surfaces have been developed and perform well in the nearfield where buoyant forces clearly dominate spreading due to atmospheric turbulence. Additional research is required for determining concentrations in the transition zone between dominance by buoyant forces and turbulent mixing.

The model presented consists of two components, a negatively buoyant cylindrical spreading model and a passive dispersion model. The initial spreading of the dense cloud is controlled by gravitational effects, and the cloud essentially slumps under the influence of gravity. Slumping is terminated by entrainment of air. This results in a dense gas cloud which hugs the ground as it travels downwind. Eventually the cloud of dispersing gas becomes dilute, and atmospheric turbulence dominates the cloud growth. Van Ulden (1974) recommends ending the slumping phase when the frontal velocity becomes less than twice the friction velocity. At this point, the maximum spread radius is calculated. This radius is approximate since the simple spreading model of Van Ulden neglects any entrainment during the slumping phase.

To approximate dilution due to entrainment, a relationship is defined which estimates the volume to be added to the cloud as a result of edge entrainment. This total volume is then used to calculate the cloud height at the termination of spreading. The entrainment parameter for edge spreading is given by Cox and Carpenter (1980). Gravitational spreading is assumed to occur instantaneously and to be centered at the initial source location. The resultant cloud is assumed to be cylindrical with dimensions given by the maximum spread radius and height determined from the spread volume.

Dispersion under the control of atmospheric turbulence is assumed to be represented by a passive Gaussian volume source model. Virtual distances are calculated using expressions similar to those presented in Section 5.5.2.

Procedure:

Steps in the heavy gas simulation are shown in Flowchart D-6.

1) The maximum spread radius (m) is given by the following equation using information on the initial cloud size, density, and wind speed:

$$R_{\text{max}} = \frac{14.7}{u} \sqrt{\frac{\rho_g - \rho_a}{\rho_a}} V_0$$

 \boldsymbol{V}_{O} is determined from the initial mass released and cloud density.

2) The total cloud volume (V_T) is calculated based on the maximum radius and an approximate equation representing the final cloud volume due to edge entrainment (V):

$$V = V_{O} \left(\frac{Rmax}{R_{O}}\right)^{1.2}$$

$$V_{T} = V_{O} + V$$

3) Cloud height can then be calculated assuming a cylindrical shape:

$$H = \frac{V_{T}}{\pi R_{\text{max}}^{2}}$$

In the case of very heavy gases, the potential exists for unrealistically thin clouds to be formed. To bound calculations in this instance, a minimum depth of 5 cm is specified. If the calculated cloud height is less than 5 cm, this height is used in further calculations and the maximum radius is recalculated.

$$R_{\text{max}} = 2.52 \sqrt{V_{\text{T}}}$$

4) The emission amount (g) for passive calculations is obtained by multiplying the initial cloud density by the initial cloud volume.

$$Q_t = V_o \rho_g$$

5) Virtual distances for passive dispersion estimates are calculated with dispersion parameters using:

$$x_{vz} = (9.3 \text{ H}) \cdot 1.64$$

 $x_z = (x_r + x_{vz} + R_{max})$

and

$$x_{vy} = (23.26 R_{max})^{1.12}$$

$$x_y = (x_r + x_{vy})$$

Calculations proceed as in Section 5.6.5 using the mass emission amount (Q_{t}), wind speed, virtual distances and stability.

5.6.3 <u>Heavy Gas Model - Continuous Release</u>

• Applicability:

The model described is applicable to short-term ambient concentration estimates resulting from continuous elevated dense gas releases occurring at a release height of 10 m or more in flat terrain. Concentration estimates are applicable for downwind distances of no more than one kilometer.

• Inputs:

```
- contaminant emission rate (kg/s)
    - stack exit velocity (m/s)
    - stack exit temperature (K)
    stack height (m)
    - stack diameter (m)
    - wind speed at stack height (m/s)
u
    - contaminant concentration in stack exit gas (percent volume)

    exhaust gas density (kg/m³)

    - exhaust gas molecular weight (g/ g-mole)
    - contaminant molecular weight(g/g-mole)
    - receptor distance (m)
     - wind speed profile exponents (see section 3.1)
р
    - ambient air density (kg/m<sup>3</sup>)
\rho_{a}

    ambient temperature (K)

C(x) - centerline ground level contaminant concentration at
       downwind distance, x (\mu g/m^3)
```

Limitations/Assumptions

The Relief Valve Discharge (RVD) model is a screening technique applicable to denser-than-air gaseous releases. The name of the model would imply that it is only applicable to pressure relief valves. However, this is not the case and the model is applicable to screening analysis of elevated dense gas releases. The model is based on wind tunnel data and empirical relationships developed by Hoot, Meroney, and Peterka (1973) using heavy gas tracers in a non-turbulent environment. Since the wind tunnel experiments most represent stable atmospheric conditions, closely concentrations that occur under unstable or neutral conditions may be significantly overestimated. The model simulates plume rise and descent under the control of buoyant forces to provide an estimate of plume trajectory to the touchdown point and concentration at the point of touchdown. The dense gas plume rises at first due to initial upwind momentum from the stack, but then sinks due to its excess density. Eventually the plume surface. centerline strikes the ground For screening calculations, the maximum concentration should be that calculated at the point of plume touchdown. If this estimate indicates a problem, more refined techniques such as the DEGADIS model should be used.

• Procedure:

The RVD model is available on a PC compatible diskette from: Source Receptor Analysis Branch, MD-14, USEPA, RTP, NC 27711. The use of this computer model is suggested for accuracy. The following is an abbreviated version of the RVD model for use as an illustrative tool only.

1) Calculate the release Richardson number R_i as described in Section 5.1.2. If $R_i \geq 30$, then dense gas effects are considered. Proceed to step 2 below.

2) Calculate Froude number, Fr:

$$Fr = u \left(\frac{\left(\frac{\rho_0}{\rho_0 - \rho_a} \right)}{9.8 \text{ d}} \right)^{0.5}$$

3) Calculate plume rise, Δh :

$$\Delta h = 1.32 \left(Fr^2 \frac{v_s \rho_0}{u \rho_a} \right)^{1/3} d$$

4) Calculate dilution ratio at maximum plume height:

$$R = 5.67 \times 10^{-2} \left(\frac{yd^2uM}{QT_a} \right) \left(\frac{\Delta h}{d} \right)^{1.85}$$

5a) Calculate plume molecular weight at maximum plume height:

$$M_{H} = \frac{M + 29 (R-1)}{R}$$

5b) Calculate density difference at maximum plume height:

$$\Delta = \frac{M_{\text{H}}^2}{29 \left[M_{\text{H}} - \frac{M \left(T_{\text{a}} - T_{\text{s}}\right)}{T_{\text{a}}R}\right]} - 1$$

If Δ < 0.005, use continuous dispersion model for non-dense gases, Section 5.6.4.

6) Calculate distance at plume touchdown, x_T:

$$x_{T} = \frac{dFr^{2}u}{v_{s}} + 0.56 d Fr \left\{ \left(\frac{\Delta h}{d} \right)^{3} \left[\left(\frac{2\Delta h + h_{s}}{\Delta h} \right)^{3} - 1 \right] \left(\frac{v_{s}\rho_{a}}{u\rho_{o}} \right) \right\}^{0.5}$$

7) Calculate concentration at plume touchdown, $C(x_T)$:

$$C(x_T) = 3.1 \times 10^9 \frac{Q}{ud^2} \left(\frac{2\Delta h + h_s}{d}\right)^{-1.95}$$

8) Downwind concentrations after plume touchdown depend on critical distance, x_c :

$$x_{c} = x_{T} \left(\frac{2.045 \times 10^{5} \cdot M_{c}}{C(x_{T})} \right)^{-1.538}$$

If
$$x_C < x_T$$
, let $x_C = x_T$.

If receptor distance $x < x_c$:

$$C(x) = C(x_T) \left(\frac{x}{x_T}\right)^{-0.65}$$

If receptor distance $x \ge x_C$:

$$C(x) = C(x_T) \left(\frac{x_C}{x_T}\right)^{-0.65} \left(\frac{x}{x_C}\right)^{-1.7}$$

Model results should be reviewed first to determine if the plume touches down within 1 kilometer. If it does, then an estimate of touchdown distance and concentration is available. If touchdown is not indicated within the first kilometer, the model is performing beyond its scope.

5.6.4 Dispersion Model for Continuous Releases

• Applicability:

Simulations of dispersion from continuous point sources and continuous area or volume sources through application of virtual point source techniques. May also be applied to sources with wake effects due to building downwash.

• Inputs:

Q - emission rate (g/s) σ_z , σ_y - continuous vertical and horizontal dispersion parameters (m)

u - wind speed (m/s)

• Limitations/Assumptions:

- Method provides centerline maximum concentrations with downwind distance for specific input conditions.

• Reference:

- Turner (1970)

• Procedure:

Concentrations in g/m^3 are provided at each downwind distance, x, by the following equation.

$$C(x) = \frac{Q}{\pi \sigma_z \sigma_y u} \left[exp -0.5 \left(\frac{H}{\sigma_z} \right)^2 \right]$$

The effective dispersion parameters incorporate, where necessary, initial dispersion due to wake effects as well as area or volume source releases. Concentrations estimated represent one hour average values.

5.6.5 Dispersion Model for Instantaneous Releases

• Applicability:

Simulations of dispersion from instantaneous point sources and continuous volume or area sources through application of virtual point source techniques.

• Input:

Qt - release amount (g) H - effective source height (m)

 σ_z , σ_y - instantaneous horizontal and vertical dispersion parameters (m)

• Limitations/Assumptions:

- Maximum ground level concentrations are provided for the center of each instantaneous puff at selected downwind locations.
- Full surface reflection is assumed.
- Crosswind and downwind dispersion are assumed to be equal.
- The downwind position of the puff is determined by multiplying wind speed times travel time.

• Reference:

- Petersen (1982)

• Procedure:

- 1) Use of the PUFF model (Petersen, 1982) will simplify calculations.
- 2) Hand calculations are provided by:

$$C = \frac{0.127 \text{ Qt}}{\sigma_z \sigma^2_y} \quad \exp \left(-0.5 \left(\frac{\text{H}}{\sigma_z}\right)^2\right)$$

The technique is strictly valid only if travel time to the receptor from the source exceeds the release duration. Otherwise, an unrealistically high concentration will result.

6.0 EXAMPLES

This section provides examples for the release scenarios identified in Table 2-1 and Section 4. These examples illustrate the solution to mathematical equations used in the text and may not represent the maximum short-term ground level concentration estimate from a meteorological perspective. To obtain these maximum concentrations, the user should follow the procedures outlined in Section 2.4.

6.1 Continuous Gaseous Emissions from Stacks

Scenario: Hydrocyanic Acid (HCN) is released from a vent stack. Hourly maximum concentration estimates are required.

<u>Discussion</u>: This example represents a continuous stack release of a vapor or, similarly, particulate matter at near ambient conditions. The only difference for particulate matter is that plume density checks would not be performed. In the example, flow is under the influence of a nearby building. Emission rates are determined as specified in Section 4.1.2 and shown in Flowchart C-5. Emission rates must be calculated from process parameters or determined from representative emission factors. In this case, emissions are specified. Emission factors are also available (see Appendix A). Dispersion procedures are outlined beginning in Flowchart D-1.

6.1.1 Building Cavity Example

Source Parameters

 $M_{HCN} = 27 \text{ g/g-mole}$ $T_a = 298 \text{ K}$ $T_s = 298 \text{ K}$ d = 0.1 m $V = 0.14 \text{ m}^3/\text{s}$

 X_{rec} = distance to property line = 25 m Q = 9.3 x 10⁻⁴ g/s

 $h_s = 16 m$

 h_b = height of building = 19 m

L = alongwind building dimension = 19 m W = crosswind building dimension = 19 m

L_b = lesser dimension = 19 m

 $v = \text{stack exit velocity} = 4V/(\pi d^2) = 17.8 \text{ m/s}$

Sample Estimates

1) (Flowchart D-1 and Section 5.1.2). Because HCN (molecular weight 27) is the primary constituent (besides air) in the gas stream, and its concentration is low compared to air, the overall molecular weight of the gas stream can be approximated by that of air. Alternatively, mean density calculations would show the gas stream to have a mean molecular weight which is slightly less than air.

$$M_S = 28.9 \text{ g/g-mole}$$

2) Determine if dispersion is affected by negative buoyancy (Section 5.1.2).

$$\frac{T_s}{M_s} = \frac{298}{28.9} = \frac{T_a}{28.9}$$

Negative buoyancy is not a factor and point source passive dispersion techniques apply (Flowchart D-2).

- 3) Determine if plume is in the cavity (Section 5.6.1)
 - Compare stack height to cavity height (Note that L_b = L = W for this square building):

$$h_C = 19 \text{ m} + 0.5 \text{ (19 m)} = 28.5 \text{ m}$$

 $h_{\rm S}$ = 16 m < $h_{\rm C}$; therefore, the stack release height is in the cavity

• Calculate the momentum flux and plume rise (Note that stack exit velocity is obtained from the volumetric flow rate and the stack diameter):

$$F_{\rm m} = \left(\frac{298 \text{ K}}{298 \text{ K}}\right) \left(17.8 \frac{\text{m}}{\text{sec}}\right)^2 \quad (0.1\text{m})^2 / 4 = 0.79 \text{ m}^4/\text{s}^2$$

$$h_{\rm m} = \left[\frac{3 (0.79 \text{ m}^4/\text{s}^2) 2 (19 \text{ m})}{(0.33 + 10 \text{ m/s}/17.8 \text{ m/s})^2 (10 \text{ m/s})^2} \right]^{1/3} = 1.0 \text{ m}$$

• Compute plume height and determine if plume is in cavity:

$$H_D = 16 m + 1 m = 17 m$$

H_D < h_C; therefore plume is in cavity

- 4) Determine if the receptor is in cavity.
 - Compute the downwind extent of the cavity

 $L/h_b = 19 \text{ m/19 m} = 1$; therefore use the equation for short buildings:

$$x_r = \frac{[-2.0 + 3.7 (19/19)^{-0.33}] 19}{1.0 + [-0.15 + 0.305 (19/19)^{-0.33}] (19/19)} = 28.0 m$$

For receptor = 25 m, receptor is in cavity region. Use cavity model (Section 5.6.1). The cavity calculation would not be necessary if the receptor were outside of the plant boundary.

A = (h_b) (L) = 19 m x 19 m = 361 m²

$$C = \frac{9.3 \times 10^{-4} \text{ g/s}}{1.5 \text{ (361 m}^2) \text{ (1 m/s)}} = 1.7 \times 10^{-6} \text{ g/m}^3 = 1.7 \text{ µg/m}^3$$

6.1.2 Near-Wake Example

In the previous example cavity calculations were required. If in the example

$$h_s = 28 \text{ m}$$

and

$$x = 100 m$$
,

an alternative path of calculations is necessary, resulting in a near-wake region concentration estimate. From step 3 above:

$$h_s = 28$$

$$H_D = 28 + 1.2 = 29.2$$

 $H_p > 28.5$ (the cavity height). Therefore, the plume is not in the cavity and the user should follow Section 5.5.3.

Sample Estimates

1) $h_w = ((19)^2 + (19)^2)^{1/2} = 26.9 \text{ m}$

Since: $h_s + h_m = 28 m + 1.1 m = 29.1 m$

and:

29.1
$$\left\{\begin{array}{l} 2.5 \ (19 \ m), \text{ or} \\ 1.5 \ (19 \ m) + 19 \ m, \end{array}\right.$$

wake effects are significant.

2) Compare receptor distance to the wake region.

$$x = 100 \text{ m} < 10 (19 \text{ m})$$

therefore, near wake equations are used.

3) In Section 5.3.3, all parameters through step 2 are calculated.
 In step 3:

$$x = 100 \text{ m} > 3 (19),$$

therefore, the receptor is located in the near wake region.

4) Calculate plume dispersion parameters:

$$x = 25 m < 10 (19)$$

therefore:

$$\sigma_z = 0.7 (19 \text{ m}) + 0.067 (100 \text{ m} - 3 (19 \text{ m})) = 16.18 \text{ m}$$

and,

$$h_s + h_m = 29.1 \text{ m} < 1.2 (28 \text{ m})$$

therefore:

$$\sigma_y = 0.35 (19 \text{ m}) + 0.067 (100 \text{ m} - 3 (19 \text{ m})) = 9.53 \text{ m}$$

5) Calculate concentration using Section 5.6.4:

C (100 m) =
$$\frac{9.3 \times 10^{-4} \text{ g/s}}{3.14 \text{ (9.53 m) (16.18 m) 1 m/s}} \exp \left[-0.5 \left(\frac{29.1}{16.18}\right)^2\right]$$
$$= 3.81 \times 10^{-7} \text{ g/m}^3 = 38.1 \text{ µg/m}^3$$

6.1.3 Far-Wake Example

The far-wake region is defined as receptor distances beyond 10 h_a or, in this example, $x \ge 190$ m. This section demonstrates a calculation for a receptor at 200 m from the source.

Sample Estimates

1) The far-wake determination is made in Section 5.5.3, Step 3. In Step 4, dispersion parameters are calculated along with virtual distances:

$$\sigma_{\rm V}$$
 = 0.82 (19 m) = 15.6 m

$$\sigma_z = 1.2 \text{ (19 m)} - 22.8 \text{ m}$$

giving virtual distances using Figures 5-1 and 5-2 (stability F):

$$x_{VV} = 440 \text{ m}$$

$$x_{772} = 2200 \text{ m}$$

2) In Section 5.3.3, check the location of the receptor relative to the cavity zone. The dispersion parameters are determined using virtual distances, x_{VY} , x_{VZ} (stability F):

$$\sigma_{V}$$
 (200 m + 440 m) = 22 m

$$\sigma_z$$
 (200 m + 2200 m) = 24 m

3) Calculate concentration (Section 5.6.4):

C (200 m) =
$$\frac{9.3 \times 10^{-4} \text{ g/s}}{3.14 \text{ (22 m) } 24 \text{ m (1 m/s)}} = \exp \left[-0.5 \left(\frac{29.2 \text{ m}}{24 \text{ m}}\right)^2\right]$$

$$= 2.68 \times 10^{-7} \text{ g/m}^3 = 26.8 \text{ }\mu\text{g/m}^3$$

6.2 Fugitive Dust

Scenario: Concentration estimates at the fenceline are required for arsenic emissions resulting from wind erosion from a pile of flyash at a secondary lead smelter blast furnace.

<u>Discussion</u>: This example demonstrates calculation of particulate emissions from storage piles and use of particulate matter profiles to study a specific toxic chemical. Maximum concentration estimates are normally obtained using the procedures described in Section 2.4. Worst case estimates, in this case, use conservative assumptions and deviate from those discussed in Section 4.2 since maximum emissions are wind speed dependent.

Source Parameters

Ash pile: height - 3 m diameter - 10 m

Distance to boundary 100 m

Sample Estimates

1) The fugitive dust scenario is presented in Section 4.2, and estimates follow Flowchart C-2. Fugitive emissions for this scenario are not directly available. Emissions factors for aggregate storage are available in AP-42 as are particulate matter profiles (Appendix A). For this example, the profiles indicate that arsenic makes up 0.3 percent of fine particles (less than 2.5 microns) emissions mass. The aggregate storage emission factor for windblown dust is:

E (kg/day/hectare) = 1.9 (s/1.5)
$$\frac{(365-p)}{235}$$
 (f/15)

where:

s - percent silt content

p - number of days with more than 25 mm of precipitation

f - percent of time wind exceeds 5.4 m/s

Since the factor is not directly applicable, conservative assumptions are made that 20 percent of wind exceeds 5.4 m/s, no days have precipitation in excess of 25 mm and the silt content is 50 percent. The calculated emission rate is 131.2 kg/day/hectare

or 0.00015 g/(s m²). Since 0.3 percent of this mass is arsenic, the emission rate is 4.55 x 10^{-7} g/(s m²) over 78.5 m² (π r² area) or 3.58 x 10^{-5} g/s.

2) The pile height is relatively low (3 m) in height, and conservative estimates will result if area source techniques (Flowchart D-4) are used. The initial horizontal plume spread parameter is given by (Section 5.5.1):

$$\sigma_{v} = 10 \text{ m/4.3} = 2.3 \text{ m}$$

3) Meteorological conditions resulting in maximum concentrations for a ground level area source are low wind speed (1 m/s), stable (F) conditions. These are assumed for conservatism and provide a virtual distance from Figure 5-1 of approximately:

$$x_v = 74 \text{ m}$$

4) Using this distance with the minimum receptor distance, the horizontal and vertical dispersion parameters (Section 5.3.1) are determined from Figures 5-1 and 5-2:

$$\sigma_{y}$$
 (174 m) = 6.6 m
 σ_{z} (100 m) = 2.3 m

5) Maximum estimated concentration is obtained from Section 5.6.4 (the exponential term equals unity because H is zero):

$$C = \frac{3.58 \times 10^{-5} \text{ g/s}}{3.14 \text{ (6.6 m) } 2.3 \text{ m (1 m/s)}} = 7.5 \times 10^{-7} \text{ g/m}^3 = 0.75 \text{ µg/m}^3$$

6.3 Instantaneous Ejection of Particles from Ducts

Scenario: A failure of a pneumatic conveyor system carrying 3,3-dichlorobenzidine powder from a spray dryer lasted 5 minutes. Estimates are required for 15-minute average concentrations at receptors greater than 100 m downwind of the source.

<u>Discussion</u>: The scenario represents a class of possible releases from various types of gas-solid conveyance systems or reactor failures. Common causes of this type of release are duct failures due to abrasion or failure of flexible connectors. Short duration events can be simulated as instantaneous passively dispersing puffs (i.e., all mass was released instantaneously (within one minute)). The effect of this assumption is a conservative concentration estimate. In general, powders emitted by this type of release will consist of relatively large particles (order of 10 microns) which would be subject to gravitational fallout. Since the screening techniques neglect deposition and fallout, conservative concentration estimates are expected.

Source Parameters

release height = 10 m conveyance rate = 2 kg/s duct diameter = 0.305 m

Sample Estimates

1) Section 4.3 and Flowchart C-3 indicate that duct failure emissions are typically user estimated and that dispersion calculations follow point source procedures in Flowchart D-6 (a point source is assumed because no indication of initial dilution dimensions are provided in the problem). The release scenario would result in an initially high rate of emissions which decreases rapidly as line pressure decreases, as in a pipeline blowdown. One example of a user calculation is given by assuming that total emissions (Q_t) consist of that material which would normally be conveyed in a 5 minute period, i.e.:

$$Q_t = (5 \text{ minutes}) \left(\frac{60 \text{ s}}{\text{min}}\right) 2 \text{ kg/s} = 6.0 \times 10^5 \text{ g}$$

2) Since the release is at 10 m, the distance to maximum ground level concentration (Section 2.4) is approximately that at which $\sigma_z = H/\sqrt{2}$ or 7 m. Distances to maximum concentration for each stability are determined from Figure 5-4:

Stability	Distance (m)	$\sigma_{\mathbf{z}}$ (m)	σ _y (m)
unstable	30	7	3
neutral	240	7	10
stable	3500	7	30
(unstable)	(100)	(10)	(10.5)

The maximum concentration occurs where the product σ_y σ_z^2 is a minimum which, for this case, is under unstable conditions. Since the distance to maximum concentration for unstable conditions is within the minimum receptor or fenceline distance (100 m), dispersion parameters for 100 m were also determined.

3) With the unstable dispersion parameters considered, the maximum concentration occurs with the minimum product of σ_z σ_y^2 , or during neutral conditions. From Section 5.6.5:

$$C = \frac{0.127 \text{ Qt}}{\sigma_z \sigma_y^2} = \frac{0.127 (6.0 \times 10^5 \text{ g})}{7 \text{ m} (10 \text{ m})^2} = \exp(-0.5 (10 \text{ m/7 m})^2)$$

$$= 39.2 \text{ g/m}^3$$

The resultant peak 15 minute average concentration at the receptor can be found using techniques in Appendix E:

$$N = \frac{(900 \text{ s}) (1 \text{ m/s})}{2 (10 \text{ m})} = 45 \text{ giving A} = 1$$

$$F = \frac{A - 0.5}{(0.3989) 45} = 0.028$$

The concentration is then:

$$C_{avg} = 0.028 (7.85 \text{ g/m}^3) = 1.10 \text{ g/m}^3$$

6.4 Flare Emissions

Scenario: A gas is sent to an elevated flare to be burned. For simplicity, it is assumed that the flare is permitted. The gas is a mixture with one toxic component. The gas stream is made up of methane, ethane, carbon dioxide and benzene. Maximum one-hour concentrations are required for benzene assuming 98% reduction efficiency of the flare.

<u>Discussion</u>: Flare problems are done in two parts, an emission calculation and dispersion modeling. Toxic emissions for permitted flares are reduced to 2% of the potential emissions based on a required control efficiency of 98%. Flare problems are similar to stack examples except that there are buoyancy flux reductions associated with radiative heat losses and a need to account for flame length in estimating plume height. Estimates of concentrations require calculations of heat flux, flame length, plume rise and dispersion.

Source Parameters

Fi = gas composition (volume fraction):

- methane - 0.50

- ethane - 0.098

- carbon dioxide - 0.40

- benzene - 0.002

 h_s = flare height - 32 m

V = flow rate to flare - 6.58 m³/s

Sample Estimates

The flare scenario is presented in Section 4.4 and Flowchart C-4. Steps in calculations are as follows:

1) Determine the emission rate of benzene from the volume fraction, molar volume, flow rate, and molecular weight. The volume of benzene is the fraction times flow rate:

 $V(benzene) = 0.002 (6.58 m^3/s) = 0.013 m^3/s$

Mass emission rate after controls is given by determining the number of moles in the benzene fraction and multiplying times molecular weight (the gas is assumed to be at standard conditions) considering the control efficiency:

$$Q = \frac{(0.013 \text{ m}^3/\text{s}) (78.1 \text{ g/g-mole}) (0.02)}{0.0224 \text{ m}^3/\text{g-mole}} = 0.9 \text{ g/s}$$

2) Calculate the total heat release from the flare (Section 5.2.2). In this example, carbon dioxide is not combustible and is assumed not to affect flame heat. Total heat generated by the flame is determined using mole fractions, molar flow rate, and heats of combustion for methane, ethane, and benzene (see references of physical constants).

$$Q_t = (44.64 \text{ g-mole/m}^3) 6.58 \text{ m}^3/\text{s} [0.5(191,760 \text{ cal/g-mole}) + 0.098 (341,260 \text{ cal/g-mole}) + 0.002 (780,922 \text{ cal/g-mole})]$$

$$= 3.84 \times 10^7 \text{ cal/s}$$

3) Compute the flame tip height, Flowchart D-7 (Section 5.2.2):

$$h_f = 4.56 \times 10^{-3} (3.84 \times 10^7)^{0.478}$$

= 19 m

4) Calculate the effective release height before plume rise:

$$h_{se} = 32 m + 19 m = 51 m$$

5) Determine the buoyancy flux from the heat release rate (Section 5.2.3):

$$F = 1.66 \times 10^{-5} (3.84 \times 10^{7})$$
$$= 637.4 \text{ m}^{4}/\text{s}^{3}$$

6) Buoyancy plume rise calculations begin at step 3 of Section 5.2.3. The distance to final plume rise for unstable conditions and $F > 55 \text{ m}^4/\text{s}^3$ is:

$$x_f = 119 (637.4)^{0.4} = 1575 m$$

The high buoyancy of this release makes determination of the maximum concentration very complex. The distance to final plume rise at 1568 m would in most applications be well beyond the facility fenceline distances. As a

result, the potential exists for the maximum concentration to occur during the transitional plume rise stage which makes the concentration calculations very complex. That is, plume rise is a function of wind speed, downwind distance, and stability, concentration is a function of dispersion parameters, wind speed and height of release, and dispersion parameters are a function of stability and downwind distance. The method of determining maximum concentration available in Section 2.4 requires numerous iterations to determine the maximum concentration. In this instance, it is recommended that refined modeling, such as ISC, be used to determine maximum concentrations. An alternative to refined modeling or iterative solutions is the very conservative assumption that the maximum plume height equals the stack height modified by the flame length.

The following steps are included to demonstrate calculations for a single receptor distance (1 km) and arbitrary meteorological condition (5 m/s and B stability) typically required in an iteration to determine maximum concentration.

7) The receptor distance is less than x_f and is used to estimate a transitional plume rise (step 4 of Section 5.2.3):

$$\Delta h = 1.6 \frac{(637.4)^{0.33}(1000)^{0.67}}{5 \text{ m/s}} = 276 \text{ m}$$

Effective plume height is given by:

$$H = 276 m + 51 m = 327 m$$

8) Dispersion parameters (Flowchart D-3 and Section 5.3.1) for receptors at 1000 m are:

$$\sigma_{\mathbf{Y}}$$
 (1000 m) = 158 m

$$\sigma_{z}$$
 (1000 m) = 110 m

9) The effects of buoyancy induced dispersion (Section 5.4) are calculated by:

$$\sigma_{y} = [(158 \text{ m})^{2} + (276/3.5)^{2}]^{0.5} = 177 \text{ m}$$

$$\sigma_{z} = [(110 \text{ m})^{2} + (276/3.5)^{2}]^{0.5} = 135 \text{ m}$$

10) One-hour concentrations can then be calculated at the receptor by (Section 5.6.4):

$$C = \frac{0.9 \text{ g/s}}{3.14 (5 \text{ m/s})(135 \text{ m})(177 \text{ m})} \exp[-0.5(327 \text{ m/135 m})^2]$$
$$= 1.28 \times 10^{-7} \text{ g/m}^3 = 0.128 \mu\text{g/m}^3$$

6.5 Continuous Gaseous Releases from Tanks or Pipes

Scenario: In this example chlorine gas is released from the vapor space of a pressurized tank through a 2.8 cm diameter hole.

Discussion:

This scenario represents a continuous gaseous release from a pressurized vessel. The equations used in the calculations are shown in Section 4.5.

Source Parameters

Chlorine gas:- molecular weight = 70.9 g/g mole
- temperature = ambient = 283 K
- pressure = 6.89 x 10⁶ dynes/cm²
- ratio of specific heats = 1.35
minimum receptor distance = 100 m

Sample Estimates

Calculations for this release are guided by Section 4.5 and Flowchart C-6. Steps in the calculations are as follows:

1) Release calculations:

Because the release is single component, mean density and mean specific heat ratios are not required. Calculations begin with a determination of the emission rate from the leaking tank. Selection of the equation for release rate depends on the ratio of tank to atmospheric pressure:

$$\frac{P_t}{P_a}$$
 = (6.89 x 10⁶ dynes/cm² / 1.01 x 10⁶ dynes/cm²)
= 6.8

to be compared to the conditional value:

$$\left(\frac{(1.35+1)}{2}\right)^{(1.35-1)} = 1.86$$

Since the pressure ratio is greater than the conditional value of 1.86 generated using the specific heat ratio of 1.35, the critical flow equation is used after calculating vapor density by:

$$\rho_{V} = \frac{M P_{t}}{R_{*} T}$$

$$= \frac{70.9 \text{ g/g-mole } .(6.89 \times 10^6 \text{ dynes/cm}^2)}{(8.31 \times 10^7 \text{ dyne-cm/g-mole K})} = 0.0208 \text{ g/cm}^3$$

and:

$$q_v = 0.8 (6.16 \text{ cm}^2) \sqrt{(1.35)6.89 \times 10^6 \text{ dynes/cm}^2 \cdot (0.0208 \text{ g/cm}^3) \left(\frac{2}{1.35+1}\right)^{\frac{1.35+1}{1.35-1}}}$$

$$= 1261 \text{ g/s}$$

Prior to density determination (Flowchart D-1), the volume flow rate and exit velocity from the tank must be determined. Volume flow rate can be determined from the vapor density at tank conditions or, as in this case, from the molecular weight and molar volume:

$$V = \frac{1261 \text{ g/s}}{70.9 \text{ g/g-mole}} \bullet 0.0224 \frac{\text{m}^3}{\text{g-mole}} \bullet \frac{1.01 \times 10^6 \text{ dynes/cm}^2}{6.89 \times 10^6 \text{ dynes/cm}^2} \bullet \frac{283}{273} \text{ K}$$
$$= 0.06 \text{ m}^3/\text{s}$$

Exit velocity is calculated from the leak area

$$V_{s} = \frac{0.06 \text{ m}^{3}/\text{s}}{3.14 \left(\frac{0.028}{2}\right)^{2}} = 97.5 \text{ m/s}$$

2) Chlorine is substantially more dense than air which can be confirmed in the first step of Flowchart D-1 (Section 5.1.2). In the second step, a determination is made of whether the density is sufficient such that buoyant effects will dominate turbulent mixing in the atmosphere. This is done using the Richardson number:

Ri = 2722
$$\left(\frac{70.9}{28.9} - 1\right) \frac{0.06 \text{ m}^3/\text{s}}{(1 \text{ m/s})^3 0.028 \text{ m}}$$

= 8,477

The value is well in excess of 30 indicating the importance of heavy gas modeling and the RVD model (Section 5.6.3) is used.

Table 6-1 provides results for this example beginning with a listing of model inputs for the version available in August, 1988. The second portion of the output identifies those cases in which the model is applicable. In this section, a "0" indicates that the release is passive and the model is inapplicable, a "1" indicates that the gas is influenced by gravitational effects and a "2" indicates that the meteorological condition identified is not likely to occur. The determination of whether the gas is affected by gravitational effects is made based initially on Richardson number for which a table is presented. Model results are given in two forms, a table showing plume rise, touchdown distance, and touchdown concentration for each meteorological condition and a table of concentrations at specified receptors. In this example both of these tables are reviewed to determine the maximum concentration. Since the fenceline is at 100 m, a review of touchdown distances in excess of 100 m indicates that the maximum concentration is 8.22 g/m³ and occurs at 125 m from the source within stability classes E and F and 2 m/s winds. A review of the table giving the post-touchdown concentration confirms that this concentration exceeds any fenceline value.

TABLE 6-1

RVD MODEL RESULTS: CHLORINE GAS LEAK

Chlorine Leak Example 08-05-1988

Input Data

Pollutant emission rate (kg/sec) = 1.261 Exit gas velocity (m/sec) = 97.6Exit Temperature (K) = 283Stack Height (m) = 5 Diameter (m) = .028Pollutant Concentration (volume %) = 100 Exhaust Gas Density (kg/m3) = 3.045529Exhaust Gas Molecular Weight = 70.9 Exhaust Gas Mass Flow Rate (kg/sec) = 1.261 Pollutant Molecular Weight = 70.9 Molar Volume (m3/mole) = 2.328003E-02Release duration (sec) = 900 Av. Time (sec) = 900 Wind Speeds (m/sec) = 1.0 2.0 4.0 6.0 8.0 10.0 Distance (m) = 100Ambient Temperature (K) = 283 283 283 283 283 283 Wind Speed Profile Exponents = .15 .15 .2 .25 .3 .3 (Friction Velocity) / (Wind Speed at z=10m) =

0.06 0.06 0.06

Dense Gas Behavior

Stability Class

Wind	1	2	3	4	5	6
Speed						
1.0	1	1	1	1	2	1
2.0	1	1	l	1	1	1
4.0	2	1	1	1	1	2
6.0	2	2	1	1	2	2
8.0	2	2	1	1	2	2
10.0	2	2	1	1	2	2

0.06 0.06

^.06

(0=Non-Dense Behavior l=Dense Gas Behavior 2=Combinations that cannot occur)

Release Richardson Numbers

Stability Class

Wind	1	2	3	4	5	6
Speed						
1.0	64534.0	64534.0	66809.8	69165.8	71604.9	71604.9
2.0	8066.7	8066.7	8351.2	8645.7	8950.6	8950.6
4.0	1008.3	1008.3	1043.9	1080.7	1118.8	1118.8
6.0	298.8	298.8	309.3	320.2	331.5	331.5
8.0	126.0	126.0	130.5	135.1	139.9	139.9
10.0	64.5	64.5	66.8	69.2	71.6	71.6

TABLE 6-1

RVD MODEL RESULTS: CHLORINE GAS LEAK

Dense Plume Trajectory

Stability Class	Wind Speed (m/sec)	Rise	Touchdown Distance (m)	Touchdo Concentra (ug/m3)	
1	1.0 2.0	9.2 7.3		0.11042E+08 0.77962E+07	0.38158E+04 0.26940E+04
2 2 2 2	1.0 2.0 4.0	9.2 7.3 5.8	65.85 140.79 305.06	0.11042E+08 0.77962E+07 0.53969E+07	0.38158E+04 0.26940E+04 0.18649E+04
3 3 3 3 3 3	1.0 2.0 4.0 6.0 8.0 10.0	9.3 7.4 5.9 5.1 4.7	63.41 135.50 293.39 464.18 644.90 833.93	0.11231E+08 0.79366E+07 0.54998E+07 0.43939E+07 0.37293E+07 0.32747E+07	0.38809E+04 0.27426E+04 0.19005E+04 0.15183E+04 0.12887E+04 0.11316E+04
4 4 4 4 4 4	1.0 2.0 4.0 6.0 8.0 10.0	9.4 7.5 6.0 5.2 4.7 4.4	61.07 130.41 282.18 446.24 619.76 801.20	0.11422E+08 0.80792E+07 0.56044E+07 0.44804E+07 0.38045E+07 0.33420E+07	0.39470E+04 0.27918E+04 0.19366E+04 0.15482E+04 0.13147E+04 0.11548E+04
5 5	2.0 4.0	7.6 6.0	125.52 271.40	0.82239E+07 0.57106E+07	0.28418E+04 0.19734E+04
6 6	1.0	9.6 7.6	58.81 125.52	0.11616E+08 0.82239E+07	0.40141E+04 0.28418E+04

TABLE 6-1

RVD MODEL RESULTS: CHLORINE GAS LEAK

Concentrations at Specific Receptor Distances

Stability Class		Distance	Concentration	
C1055	-	(m)	(ug/m3)	(ppm)
1	1.0	100.0	0.54271E+07	0.1875E+04
2	1.0	100.0	0.54271E+07	0.1875E+04
3	1.0	100.0	0.51773E+07	0.1789E+04
4	1.0	100.0	0.49390E+07	0.1707E+04
	~			
6	1.0	100.0	0.47117E+07	0.1628E+04

6.6 Instantaneous Gas Releases

Scenario: An instantaneous chlorine discharge results from failure of a transfer line from a pump. An instantaneous chlorine cloud is formed for which an estimate of the peak concentration at 100 m from the release is required.

<u>Discussion</u>: This scenario represents any instantaneous gas release which may result from a vent, stack, pipe or compressor failure, relief valve or similar case. Dispersion estimates require characterization of the cloud primarily to determine if calculations should be made using a dense or passive model. Calculations are guided by Section 4.6 and Flowchart C-7.

Source Parameters

- release temperature - 283 K
- molecular weight 70.9 g/g-mole
- ambient temperature 283 K
- transfer line: diameter 2 cm
 length in release region 3 m

Sample Estimates

1) Because the release is single component, calculations of mean values do not apply. Begin by calculating the mass released from the known volume. In other cases, release mass may be known and volume will be determined. In this example, it is conservatively assumed that all gas in the isolated pipe segment is available instantaneously as an emission input to a dispersion model. From volume considerations:

$$V_i = 3 \text{ m} (3.14 (0.02/2)^2) = 0.0009 \text{ m}^3$$

The release mass is determined using either a known density or, in this case, the molar volume and molecular weight.

$$Q_t = \frac{(0.0009 \text{ m}^3)(70.9 \text{ g/g-mole})}{0.0224 \text{ m}^3/\text{g-mole}} = \frac{283 \text{ K}}{273 \text{ K}} = 2.95 \text{ g}$$

2) Calculate Richardson number as a check on puff density. The Richardson number is given by:

Ri = 2,722
$$\left(\frac{70.9 \text{ g/g-mole} \cdot 283 \text{ K}}{28.9 \text{ g/g-mole} \cdot 283 \text{ K}} - 1\right) \frac{.0009 \cdot 0.33}{(1 \text{ m/s})^2} = 391$$

which indicates dense gas modeling should be used.

3) Steps in the heavy gas simulation are given in Flowchart D-6 (Section 5.6.2):

$$Rmax = \frac{14.7 (1.45 (0.0009 m^3))^{0.5}}{1 m/s} = 0.53 m$$

where 1.45 is the ratio of the density difference to the density of air. This is identical to the parenthetical expression in Step 2.

Initial conditions for releases of the type must be assumed. In this case it is assumed that the gas released forms a hemisphere. An initial radius for the cylindrical heavy gas model is determined by equating the hemispherical and cylindrical volumes and assuming the radii are equal:

$$\frac{2}{\pi r^3} = \pi r^2 h$$

so that $h = \frac{2}{3}$ r. Then, for the model

$$V_{o} = \frac{2}{3} \pi R_{o}^{3} \text{ and } R_{o} = \left(\frac{3 V_{o}}{2 \pi}\right)^{0.33}$$

The initial radius is:

$$R_{O} = \begin{bmatrix} 3 & (0.0009 \text{ m}^{3})^{0.33} \\ \hline 2 & 3.14 \end{bmatrix} = 0.077 \text{ m}$$

The entrained volume is:

$$V = 0.0009 \text{ m}^3 \left(\frac{0.53 \text{ m}}{0.077 \text{ m}} \right)^{1.2} = 0.009 \text{ m}^3$$

$$v_T = 0.0009 \text{ m}^3 + 0.009 \text{ m}^3 = 0.0099 \text{ m}^3$$

and:

$$H = \frac{0.0099 \text{ m}^3}{3.14 (0.53 \text{ m})^2} = 0.0112 \text{ m}$$

4) H is less than 5 cm so $R_{\mbox{\scriptsize max}}$ is recalculated:

$$R_{\text{max}} = 2.52 \sqrt{0.0099 \text{ m}^3} = 0.25 \text{ m}$$

- 5) The release is sufficiently small such that the initial spread radius is trivial relative to turbulent spreading and calculations can be completed using the simple Gaussian puff model without considering virtual distances.
- 6) Dispersion parameters for this instantaneous release are determined using Figures 5-3 and 5-4 (Section 5.3.2) at a distance of 100 m for a stability of F (as defined in Section 2.4). Peak concentration is then estimated as indicated in Section 5.6.5:

$$C = \frac{0.127 (2.95 g)}{(1.2 m)^2 0.8 m} = 0.325 g/m^3$$

6.7 Continuous Releases of Fugitive Emissions

Scenario: The maximum hourly average concentration estimate is required for ambient ethylene dichloride at a fenceline receptor 100 meters downwind from a production facility.

<u>Discussion</u>: Normal production of ethylene dichloride in vinyl chloride plants results in fugitive emissions from storage and vents. Specific sources of the emissions cannot be specified. As a result, simulations make use of emission factors to provide average emissions plantwide. These emissions are used in a continuous ground level area source dispersion model.

Source Parameters

area of emissions at the plant $-100 \text{ m} \times 100 \text{ m}$ production rate -204,000 Mg/yr in continuous operation over the year

Sample Estimates

1) Section 4.7 and Flowchart C-8 guide estimates of emissions. Emissions are obtained from emission factors published by EPA (1987b). Plant-wide emissions are calculated from the production rate and an emission factor from various fugitive sources. The emission factor per production unit is given by:

chlorination vent	0.0216 kg/Mg
column vents	0.06 kg/Mg
process storage vents	0.0003 kg/Mg
process fugitive	0.265 kg/Mg
Total	0.3469 kg/Mg

Total emissions for the plant are given by:

$$q = 204 \times 10^3 \text{ Mg/year} (0.3469 \text{ kg/Mg}) = 70.77 \times 10^3 \text{ kg/year}$$

= 2.24 g/s

2) Dispersion estimates are provided by calculations using continuous area source equations (Flowchart D-4). Fugitive emissions are generally assumed to be dilute and therefore not dense. The virtual source distance (Section 5.5.1) using the width of the square plant area is:

$$\sigma_{v} = W/4.3 = 100 \text{ m}/4.3 = 23.2 \text{ m}$$

From Figure 5-1 , under stable (F) conditions:

$$x_v = 620 \text{ m}$$

and:

$$x_y = (620 + 100 m) = 720 m$$

for receptors at 100 m.

3) Concentrations are calculated using Section 5.6.4:

$$C = \frac{Q}{\pi \sigma_z (100 \text{ m}) \sigma_y (720 \text{ m}) u} \exp (-0.5 (H/\sigma_z)^2)$$

Since the source is at ground level, H=0 and the exponential term =1

$$C = \frac{2.24 \text{ g/s}}{3.14 (2.3 \text{ m}) 25 \text{ m} (1 \text{ m/s})} = 1.24 \times 10^{-2} \text{ g/m}^3$$

6.8 Continuous Gaseous Emissions from Land Treatment

Scenario: Sludge containing 1000 ppm benzene is applied to a one acre land treatment site at a rate of 1 lb/ft² and filled to a depth of 8 inches. Determine the one-hour average concentration of benzene 200 m downwind during the first one hour after application. The following input data are known or assumed:

```
D = 0.027 cm<sup>2</sup>/s

P = 0.1244 atm

MW_{oil} = 142 g/g-mole (assumed to be decane)

M = 1 1b/ft<sup>2</sup> = 0.489 g/cm<sup>2</sup>

h_p = 8 in = 20.3 cm

R = 82.06 cm<sup>3</sup> • atm/g-mole • k

T = 298 K

t = 3600 sec

ppm = 1000 g benzene/10<sup>6</sup> g oil

A = 1 acre = 40,468,564 cm<sup>2</sup>

x_r = 200 m fenceline distance
```

<u>Discussion</u>: Simulations of emissions from land treatment are handled using the procedures specified in Section 4.8 and release Flowchart C-9. The resultant emission rate, along with the area of the land treatment operation, is then used to determine virtual distance, dispersion rates, and receptor concentration, as outlined in Flowchart D-4.

Sample Estimates

1) Average emissions over first hour after application are estimated using the equation of Section 4.8:

$$E = \left(\frac{(0.027 \text{ cm}^2/\text{s})(0.1244 \text{ atm})(142 \text{ g/g-mole})(0.489 \text{ g/cm}^2)}{5(20.3 \text{ cm})(82.06 \text{ cm}^3 \text{ atm/g-mole} \cdot \text{K})(298 \text{ K})(3600 \text{ s})}\right)^{0.5} \cdot (1000 \text{ ppm}) \cdot (40,468,564 \text{ cm}^2) \cdot 2 \times 10^{-6}$$

$$E = 0.414 \text{ g/s}$$

- 2) As indicated in Flowchart D-4, dispersion from land treatment emissions is treated as a continuous, passive area source. The virtual horizontal distance (Section 5.5.1), based on the equivalent square dimension of the facility, is used to determine horizontal dispersion.
 - estimate σ_{VO}

$$W = (40,468,564 \text{ cm}^2)^{0.5} = 6361 \text{ cm} = 63.6 \text{ m}$$

 $\sigma_{VO}(W) = 63.6 \text{ m}/4.3 = 14.8 \text{ m}$

• determine the horizontal virtual distance x_V , using σ_{VO} and Figure 5-1 (assume stable conditions to ensure peak concentrations from the ground level source)

$$x_v = .41 \text{ km} = 410 \text{ m}$$
 (F stability)

ullet calculate receptor plus virtual distance, $\mathbf{x}_{\mathbf{y}}$

$$x_{y} = 200 \text{ m} + 410 \text{ m} = 610 \text{ m}$$

- 3) Calculate dispersion parameters (Section 5.3.1) and receptor concentration (Section 5.6.4)
 - determine σ_y at the modified horizontal receptor distance, x_y (Figure 5-1)

$$\sigma_{v}$$
 (610 m) = 21 m (F stability)

• determine σ_z at the receptor distance (Figure 5-2)

$$o_z$$
 (200 m) = 4 m (F stability)

• determine receptor concentration

$$C = \frac{0.414 \text{ g/s}}{\pi (21 \text{ m})(4 \text{ m})(1 \text{ m/s})}$$

$$C = 0.00157 \text{ g/m}^3$$

6.9 Municipal Solid Waste Landfill

Scenario: Hourly concentration estimates are required for emissions of perchloroethylene from a municipal landfill in Ohio.

<u>Discussion</u>: Concentration estimates from landfills are determined using either emission factors, an emissions model or site-specific measurements (Flowchart C-10). In this example, measurements are not available and the VOC emission model in Section 4.9 is used. Once VOC emissions are calculated, VOC emissions profiles (Appendix A, item 4) are used to determine what fraction of the total is perchloroethylene. Dispersion calculations use a continuous ground-level area source.

Source Parameters

- Amount of Refuse 3.8 million tons
- Landfill area 3 hectares $(30,000 \text{ m}^2)$
- Distance to nearest offsite receptor (100 m)

Sample Estimates

1) From Flowchart C-10 and Section 4.9, emissions are calculated as:

$$E(g/s) = (1 (g/s)/million tons) 3.8 million tons = 3.8 g/s$$

From the emissions profiles, perchloroethylene constitutes 0.3 percent of total VOC emissions or 0.011 g/s.

2) Dispersion estimates use the virtual point source, area approach with initial horizontal dispersion (Section 5.5.1) given by:

$$\sigma_{VO} = (30,000 \text{ m}^2)^{0.5}/4.3 = 40.3 \text{ m}$$

which, under stable conditions, results in a virtual source distance of approximately 1,200 m using Figure 5-1.

3) Dispersion parameters (Section 5.3.1) are obtained from Figures 5-1 and 5-2:

$$\sigma_{v}$$
 (100 m + 1,200 m) = 44 m

$$\sigma_z$$
 (100 m) = 2.3 m

4) The maximum estimated concentration (Section 5.6.4) is calculated from:

$$C = \frac{0.011 \text{ g/s}}{3.14 \text{ (44 m) (2.3 m) 1 m/s}} = 3.46 \times 10^{-5} \text{ g/m}^3$$

6.10 Continuous Emissions from an Herbicide

Scenario: 2,4-DB butoxy ethanol ester, a restricted herbicide, is applied to a farm field of four acres. Maximum post-application one-hour average concentrations are to be estimated. The property boundary is located 100 m from the edge of the study field.

<u>Discussion</u>: Pesticide/herbicide dispersion estimates can usually be obtained by using an emission factor and a ground-level, area source dispersion model. Emission factors are often difficult to obtain but may be available from the technical literature or state agricultural agencies. Unless emissions estimates are sensitive to meteorological conditions, maximum short-term calculations will be controlled by dispersion. The worst dispersive conditions for ground level area sources occur under low wind speed, stable conditions.

Source Parameters

field size - 14 acres (approx. 56,660 m²)

Sample Estimates

Section 4.10 and Flowchart C-11 indicate that emission factors must be specified since the evaporation rates of herbicides vary widely based on composition and sources for emission factors are not generally available. The following provides an example from a typical data source. The best emissions estimates for 2,4-DB butoxy ethanol ester were found in results of inventory and flux studies performed by the California Department of Food and Agriculture, a typical data source. In one study, they determined that half of the applied pesticide consisted of the active ingredient. Losses through evaporation were approximately equal for the first two months after

application at a rate of approximately one third of the applied material per month. Biodegradation and sequestration were not found to be significant. In the sample study, data were provided on total regional application, application rate and acreage of application. An emission factor of approximately 1.2 lb active ingredient per acre per month or 1.87×10^{-4} g/h-m² was also determined.

1) Total emissions for this example are given by the emission factor times the field area:

$$q = 56,660 \text{ m}^2 (1.87 \text{ } 10^{-4} \text{ g/h-m}^2) = 10.6 \text{ g/h} = 2.9 \text{ x } 10^{-3} \text{ g/s}$$

2) Flowchart D-4 indicates that concentration estimates for this example are made with passive area source dispersion equations. Worst case meteorology for area source estimates is represented by low wind speeds, stable (F) conditions. For this example a virtual source distance (Section 5.5.1) for a square field is given from:

$$W = (56,660 \text{ m}^2)^{0.5} = 238 \text{ m}$$

resulting in:

$$\sigma_{VO} = 238 \text{ m} / 4.3 = 55 \text{ m}$$

From Figure 5-1, the distance at which a stable horizontal dispersion parameter is 55 m is:

$$x_v = 1700 \text{ m}$$

To determine the centerline concentration at 100 m from the field edge:

$$x_y = (x_r + x_v)$$

= (219 m +1700 m) = 1919 m

where x_r includes the distance from the field center to the edge summed with the distance to the property line (100 m)

3) The horizontal dispersion parameter is determined from Figure 5-1 (Section 5.3.1).

$$\sigma_{v}$$
 (1919 m) = 62 m

The vertical dispersion parameter is determined at the receptor distance from Figure 5-2.

$$\sigma_{z}$$
 (219 m) = 4.4 m

4) Concentration (Section 5.6.4) is given by (with H = 0):

$$C = \frac{Q}{\pi \sigma_z(219 \text{ m}) \sigma_y(1919 \text{ m}) \text{ u}}$$

$$= \frac{2.9 \times 10^{-3} \text{ g/s}}{3.14 (4.4 \text{ m}) (62 \text{ m}) 1 \text{ m/s}} = 3.39 \times 10^{-6} \text{ g/m}^3$$

6.11 Equipment Openings

Scenario: A common source of emissions due to equipment openings is found in the production of coke where opening of the ovens at the completion of processing results in a near instantaneous release. One toxic component of the emissions is toluene. It is desired to estimate a 15 minute average concentration at distances beyond 50 m downwind of the source.

<u>Discussion</u>: Emissions from coke ovens result primarily from charging and discharging operations and fugitive losses which occur on a continuous basis. The example presented is for the near instantaneous emissions which result from discharging the completed coke through the oven doors. Sample simulations are based on the impact of a single furnace although in real applications total emissions from a battery of ovens over time would be more typical.

Simulations require determination of an emission factor for the oven and the total emissions based on oven capacity. Dispersion estimates are made assuming that the release is instantaneous and within the wake cavity formed by the oven battery.

Source Parameters

Sample Estimates

1) Section 4-11 and Flowchart C-12 guide the user through typical calculations for equipment openings. To begin, the emissions are estimated using emission factors (EPA, 1987b). Total toluene emissions from coke production are 0.48 lb/ton (0.24 g/kg). Emissions from door openings must be approximated. From AP-42, coke pushing emissions account for approximately three percent of VOC emissions. Coke pushing emissions are then given by multiplying the emission factor times the production rate:

2) Flowchart D-6 shows the path for dispersion estimates if the release amount is known. Because the release is heated and insufficient data on component density are available, the cloud is treated as passive for this example. Estimates of volume dispersion parameters require some assumptions on the initial release dimensions (Section 5.5.2). For this example, the coke oven door dimensions are assumed:

$$\sigma_{\mathbf{Z}} = H_{\mathbf{V}}$$
 / 2.15 = 5 m/ 2.15 = 2.3 m $\sigma_{\mathbf{Y}} = W$ / 4.3 = 40 m/ 4.3 = 9.3 m

From Figures 5-3 and 5-4, under stable conditions:

$$x_{VY} = 994 \text{ m}$$
 $x_{VZ} = 542 \text{ m}$
and:
 $x_{Y} = (994 + 50 \text{ m}) = 1044 \text{ m}$
 $x_{Z} = (542 + 50 \text{ m}) = 612 \text{ m}$

for receptors at 50 m.

3) Concentrations are calculated using Section 5.6.5 (with H = 0):

$$\sigma_{y} = 9.7 \text{ m}$$
 $\sigma_{z} = 2.5 \text{ m}$

$$C = \frac{0.127 (144 \text{ g})}{2.5 \text{ m} (9.7 \text{ m})^{2}} = 0.078 \text{ g/m}^{3}$$

4) From Appendix E, the 15 minute average (assuming a 1 m/s wind speed) is given by:

$$N = \frac{(900) (1 \text{ m/s})}{2 (9.7 \text{ m})} = 46 \text{ giving A} = 1$$
and
$$F = \frac{A - 0.5}{46 (0.3989)} = 2.73 \times 10^{-2}$$

and the average peak concentration is:

$$C_{avg} = 2.73 \times 10^{-2} (0.078 \text{ g/m}^3) = 2.13 \times 10^{-3} \text{ g/s}$$

6.12 Continuous Gaseous Emissions from Surface Impoundments

Scenario: One-hour concentration estimates of benzene are desired at a receptor located 200 km downwind of a surface impoundment. The following known data are relevant to the simulation:

Source Parameters

 $C_0 = 1000 \text{ g/m}^3$

 $H = 5.5 \times 10^{-3} \text{ atm-m}^3/\text{g-mole}$

 $A = 1500 \text{ m}^2$

F = 43.7 m

D = 1.8 m

 $Q = 0.0016 \text{ m}^3/\text{s}$

 $x_r = 200 \text{ m fenceline}$

<u>Discussion</u>: Estimates of emissions from impoundments are determined using the procedures specified in Section 4.12 and Flowchart C-13. The first equilibrium constant equation is used because the Henry's Law Constant for benzene in water is available. The resultant emission rate, along with the area of the surface impoundment, is then used to determine horizontal virtual distance, dispersion rates, and receptor concentrations, as outlined in Flowchart D-4.

Sample Estimates

Emission Calculations - Quiescent Case

1) Determine the equilibrium constant with the first form of the equation:

$$K_{eq} = (40.9)(5.5 \times 10^{-3}) = 0.225$$

2) Calculate the gas phase mass transfer coefficient

$$kq = (1.26 \times 10^{-2})(1500)^{-0.055} = 0.008 \text{ m/s}$$

- 3) Determine the liquid phase mass transfer coefficient
 - determine the k₁ equation to use based on the fetch to depth ratio:

$$\frac{F}{D} = \frac{43.7 \text{ m}}{1.8 \text{ m}} = 24.3$$

ullet Based on the criteria in Section 4.12, the second k_1 equation applies:

$$k_1 = 6.84 \times 10^{-8} \frac{43.7}{1.8} + 3.35 \times 10^{-6} = 5.01 \times 10^{-6} \text{ m/s}$$

4) Calculate the overall mass transfer coefficient

$$K_q = \left(\frac{1}{5.01 \times 10^{-6}} + \frac{1}{(0.008)(0.225)}\right)^{-1} = 5.0 \times 10^{-6} \text{ m/s}$$

5) Determine the bulk concentration in the impoundment:

$$C_{L} = \frac{(0.0016 \text{ m}^{3}/\text{s})(1000 \text{ g/m}^{3})}{(5.0 \times 10^{-6} \text{ m/s})(1500 \text{ m}^{2}) + (0.0016 \text{ m}^{3}/\text{s})} = 175.8 \text{ g/m}^{3}$$

6) Calculate the area source emission rate:

$$E = (5.0 \times 10^{-6} \text{ m/s})(175.8 \text{ g/m}^3)(1500 \text{ m}^2) = 1.32 \text{ g/s}$$

Emission Calculations - Aerated Case

An aerated impoundment example is presented as a modification to the quiescent case. Assume the impoundment has a single 75 horsepower aerator (i.e., POWR = 75), aerating half the impoundment. Repeat steps 1 through 6.

7) Estimate the turbulent liquid-phase and gas-phase mass transfer coefficients.

$$k_{la} = 0.2623 (75/(1500 m^2(0.5)) = 0.0262$$

 $k_{ga} = 0.021 (75/1)^{0.4} = 0.1181$

8) The overall turbulent and complete mass transfer coefficients are given by:

$$K_t = \left(\frac{1}{0.0262} + \frac{1}{0.225 (0.1181)}\right)^{-1} = 0.0132 \text{ m/s}$$

$$K = 0.0132 (0.5) + (1-0.5) 5.0 \times 10^{-6} = 0.0066 \text{ m/s}$$

9) Emissions are calculated as:

$$E = (0.0066 \text{ m/s}) 175.8 \text{ g/m}^3 (1500 \text{ m}^2)$$

 $E = 1,740 \text{ g/s}$

Aeration provides a significantly higher emission rate.

<u>Dispersion Calculations</u>

As indicated in Flowchart D-4, dispersion from surface impoundment emissions is treated as a continuous, passive area source. The virtual horizontal distance, based on the equivalent square dimension of the impoundment, is used to determine horizontal dispersion while vertical dispersion is handled as with a point source. Concentrations are estimated with the continuous point source Gaussian equation.

The following demonstrates dispersion for the quiescent example. For the aerated impoundment, dispersion estimates will differ only by the area source emission rate.

- 1) Determine the horizontal virtual distance for the quiescent impoundment (Section 5.5.1):
 - estimate ovo:

$$W = (1500 \text{ m}^2)^{0.5} = 38.7 \text{ m}$$

$$\sigma_{yo} = \frac{38.7}{4.3} = 9 \text{ m}$$

• Determine the horizontal virtual distance, x_v , using σ_{yo} and Figure 5-1 (assume stable conditions to ensure peak concentrations from the ground level source):

$$x_v = .24 \text{ km} = 240 \text{ m}$$
 (F Stability)

calculate receptor plus virtual distance, x_v

$$x_V = 200 \text{ m} + 240 \text{ m} = 440 \text{ m}$$

- 2) Determine dispersion parameters (Section 5.3.1) and calculate receptor concentration (Section 5.6.4):
 - \bullet determine $\sigma_{Y},$ at the modified horizontal receptor distance, x_{Y} (Figure 5-1)

$$\sigma_y$$
 (440 m) = 16 m (F Stability)

ullet determine $\sigma_{\mathbf{z}}$ at the receptor distance (Figure 5-2)

$$\sigma_z$$
 (200 m) = 4 m (F Stability)

• determine receptor concentration (where H = 0)

$$C = \frac{1.32 \text{ g/s}}{\pi (16 \text{ m})(4 \text{ m})(1 \text{ m/s})}$$

$$C = 6.6 \times 10^{-3} \text{ g/m}^3$$

6.13 Relief Valve Discharge (Two-Phase)

Scenario: The relief valve scenario represents estimates of the maximum l-hour concentration resulting from a two-phase mixture of chlorine and suspended chlorine droplets.

<u>Discussion</u>: Two-phase releases can result from both relief valve discharges and liquid releases from pressurized tanks. Release estimates for relief valves must be specified, while tank releases can be calculated. The example shows the use of the RVD model for a heavy gas. Simulation using RVD requires careful definition of all input parameters to represent the density of the liquid/vapor mixture. As such, it is possible to use the one-phase RVD model to simulate aerosol (droplet) dispersion by providing as input the "equivalent" molecular weight of the aerosol mixture. However, the accuracy of such a simulation has not been evaluated.

Source Parameters

```
Chlorine gas: - molecular weight = 70.9 g/g mole
- temperature = 249 deg. K
- release rate = 3840 g/s
- exit velocity = 30.4 m/s
- exit diameter = 20 cm
- release height = 10 m
- fraction of release in liquid phase = 20 percent
nearest receptor distance = 50 m
ambient temperature = 283 deg. K
R* = 8.31 x 10<sup>7</sup> dyne cm /(g-mole K)
```

Sample Estimates

The methods for estimating concentrations for a two-phase release are presented in Section 4.13 and Flowchart C-14. Due to design differences in chemical plant processes, a generic method of obtaining emissions and release parameters is not available and these parameters must be supplied by the user.

1) Because the flashed liquid fraction is specified for this example, the first step in calculations is a determination of mean parameters of the released gas liquid/stream. The mean density in this example is given by:

$$\rho_{\rm m} = \frac{1}{(0.2/0.0034) + (0.8/3.214)}$$
$$= 0.01693 \text{ g/cm}^3$$

where (from the ideal gas law):

$$\rho_{V} = \frac{70.9 \text{ g/g-mole (1.01 x 10}^6 \text{ dynes/cm}^2)}{(8.31 \text{ x 10}^7 \text{ dyne cm/(g-mole K))}} = 0.0034 \text{ g/cm}^3$$

and from references on physical parameters:

$$\rho_1 = 3.214 \text{ g/cm}^3$$

2) An equivalent molecular weight must also be calculated:

MWe =
$$\frac{\rho_{\text{m}} R \star T}{p}$$

= $(0.01693 \text{ g/cm}^3) \left(8.31 \times 10^7 \frac{\text{dyne-cm}}{\text{g-mole K}}\right) (249 \text{ K})$
= $1.01 \times 10^6 \text{ dynes/cm}^2$

= 346.8 g/g mole

Volume release rate can be estimated using the mean density and mass rate.

$$V = \frac{q}{\rho_m} = \frac{3840 \text{ g/s}}{0.01693 \text{ g/cm}^3} = 2.27 \text{ x } 10^5 \text{ cm}^3 = 0.227 \text{ m}^3$$

3) Dispersion calculations begin with a check of the importance of buoyant effects (Flowchart D-1). A ratio test (Section 5.1.2, Step 2) indicates the plume is dense relative to air. The Richardson number test provides the same result:

Ri =
$$2722 \left(\frac{\text{Ms Ta}}{28.9 \text{ Ts}} - 1 \right) \frac{\text{V}}{\text{u}^3 \text{ d}}$$

= $2722 \left(\frac{346.8 \text{ g/g-mole } 283 \text{ deg.K}}{28.9 \text{ g/g-mole } 249 \text{ deg.K}} - 1 \right) \frac{0.227 \text{ m}^3}{(1 \text{ m/s})^3 0.2 \text{ m}}$
= $39,046$

Table 6-2 provides RVD results (Section 5.6.2) for this example beginning with a listing of model inputs. The second portion of the output identifies those cases in which the model is applicable. In this section, a indicates that the release is passive and the model is inapplicable, a indicates that the gas is influenced by gravitational effects and a "2" indicates that the meteorological condition identified is not likely to occur. The determination of whether the gas is affected by gravitational effects is made based initially on Richardson number for which a table is presented. Model results are given in two forms, a table showing plume rise and touchdown distance and concentration for each meteorological condition and a table of concentrations at specified receptors. In this example both of these tables are reviewed to determine the maximum concentration. Since the fenceline is at 50 m, a review of touchdown distances in excess of 50 m indicates that the maximum concentration is 4.26 g/m³ and occurs in stability classes B through E with 4 m/s winds at 71 m. A review of the table giving post-touchdown concentrations confirms that this concentration exceeds any fenceline value.

TABLE 6-2

RVD MODEL RESULTS: CHLORINE TWO-PHASE RELEASE

Chlorine Relief Valve Example 08-16-1988

Input Data

Pollutant emission rate (kg/sec) = 3.84Exit gas velocity (m/sec) = 30.6 Exit Temperature (K) = 249Stack Height (m) = 10 Diameter (m) = .2Pollutant Concentration (volume %) = 100 Exhaust Gas Density (kg/m3) = 17.08235Exhaust Gas Molecular Weight = 349.9 Exhaust Gas Mass Flow Rate (kg/sec) = 3.84 Pollutant Molecular Weight = 70.9 Release duration (sec) = 900 Av. Time (sec) = 900 Release pressure (atm) = 4 Wind Speeds (m/sec) = 1.0 Distance (m) = 50 4.0 6.0 8.0 10.0 2.0 Ambient Temperature (K) = 283 283283 283 283 283 Wind Speed Profile Exponents = .15 .15 .2 .25 .3 .3 (Friction Velocity) / (Wind Speed at z=10m) = 0.06 0.06 0.06 0.06 0.06 0.06

Dense Gas Behavior

Stability Class

Wind	1	2	3	4	5	6
Speed						
1.0	1	1	1	1	2	1
2.0	1	1	1	1	1	1
4.0	2	1	1	l	1	2
6.0	2	2	1	1	2	2
8.0	2	2	1	1	2	2
10.0	2	2	1	1	2	2

(0=Non-Dense Behavior l=Dense Gas Behavior 2=Combinations that cannot occur)

Release Richardson Numbers

Stability Class

Wind	1	2	3	4	5	6
Speed .		•				
1.0	38897.9	38897.9	38897.9	38897.9	38897.9	38897.9
2.0	4862.2	4862.2	4862.2	4862.2	4862.2	4862.2
4.0	607.8	607.8	607.8	607.8	607.8	607.8
6.0	180.1	180.1	180.1	180.1	180.1	180.1
8.0	76.0	76.0	76.0	76.0	76.0	76.0
10.0	38.9	38.9	38.9	38.9	38.9	38.9

TABLE 6-2

RVD MODEL RESULTS: CHLORINE TWO-PHASE RELEASE

Dense Plume Trajectory

Stability Class	Wind Speed (m/sec)	Plume T Rise (m)	Touchdown Distance (m)	Touchdo Concentra (ug/m3)	
1	1.0	13.4	13.27 32.83	0.11362E+08 0.62434E+07	0.39263E+04 0.21575E+04
2 2 2	1.0 2.0 4.0	13.4 12.6 10.0	13.27 32.83 71.84	0.11362E+08 0.62434E+07 0.42608E+07	0.39263E+04 0.21575E+04 0.14723E+04
3 3 3 3 3	1.0 2.0 4.0 6.0 8.0 10.0	13.4 12.6 10.0 8.7 7.9 7.4	13.27 32.83 71.84 114.43 159.78 207.45	0.11362E+08 0.62434E+07 0.42608E+07 0.33715E+07 0.28414E+07 0.24811E+07	0.39263E+04 0.21575E+04 0.14723E+04 0.11651E+04 0.98188E+03 0.85737E+03
4 4 4 4 4	1.0 2.0 4.0 6.0 8.0 10.0	13.4 12.6 10.0 8.7 7.9 7.4	13.27 32.83 71.84 114.43 159.78 207.45	0.11362E+08 0.62434E+07 0.42608E+07 0.33715E+07 0.28414E+07 0.24811E+07	0.39263E+04 0.21575E+04 0.14723E+04 0.11651E+04 0.98188E+03 0.85737E+03
5	2.0 4.0	12.6	32.83 71.84	0.62434E+07 0.42608E+07	0.21575E+04 0.14723E+04
6 6	1.0	13.4	13.27 32.83	0.11362E+08 0.62434E+07	0.39263E+04 0.21575E+04

TABLE 6-2

RVD MODEL RESULTS: CHLORINE TWO-PHASE RELEASE

Concentrations at Specific Receptor Distances

6 6 1.0 50.0 0.11922E+07 0.4120E+03 2.0 50.0 0.30538E+07 0.1055E+04

6.14 Two-Phase Instantaneous Release

Scenario: An instantaneous pressurized chlorine discharge results in a flash vaporization forming an instantaneous cloud of 65 percent vapor and 35 percent suspended droplets. An estimate of the peak concentration at 100 m from the release is required.

Discussion: Release estimates for two-phase instantaneous releases are beyond the scope of this workbook and data must be specified (Section 4.14 and Flowchart C-15). Techniques followed for dispersion estimates require characterization of the cloud dilution and density prior to estimates using a dense or passive model. Evaporation of droplets in the cloud cannot be simulated using the workbook. As a result, cloud density is assumed to change only by dilution.

Source Parameters

- released mass 50 kg
- molecular weight 70.9 g/g-mole
- ambient temperature 283 K
- chlorine boiling point 239 K

Sample Estimates

1) Calculate the density of the initial cloud assuming the cloud volume is attributable only to vapor and the temperature is the boiling temperature of chlorine. The vapor mass is 65 percent of total mass (50 kg) or 32.5 kg. The cloud volume is calculated from the mass of vapor using the molar volume:

$$V = \frac{32,500 \text{ g}}{70.9 \text{ g/g-mole}} \quad 0.0224 \text{ m}^3/\text{g-mole} \quad \frac{239 \text{ K}}{273 \text{ K}}$$
$$= 9.0 \text{ m}^3$$

and the mean density can be calculated as in Section 4.13 or by simple volume relationships:

$$\rho_{m}$$
 = mass/cloud volume

$$\rho_{\rm m}$$
 = 50,000 g/9.0 m³ = 5556 g/m³

2) Mean molecular weight for an instantaneous release (Section 5.1.1) is a parameter which would normally be specified. A simple calculation for this example can be performed by relating the total cloud density (vapor + droplets) and the cloud molar volume to obtain the mean molecular weight:

Ms = 5556 g/m³ (0.0224 m³/g-mole)
$$\frac{239 \text{ K}}{273 \text{ K}}$$
 = 109 g/g-mole

Richardson number is given by:

Ri = 2,722
$$\left(\frac{109 \text{ g/g-mole } 283 \text{ K}}{28.9 \text{ g/g-mole } 239 \text{ K}} - 1\right) \frac{(9.0 \text{ m}^3)}{(1 \text{ m/s})^2} = 19,481$$

which indicates dense gas modeling should be used.

3) Steps in the heavy gas simulation are given in Section 5.6.2 and Flowchart D-6:

$$R_{\text{max}} = \frac{14.7}{1 \text{ m/s}} \left[(3.46)(9.0 \text{ m}^3) \right]^{0.5} = 82 \text{ m}$$

where 3.46 is the ratio of the density difference to the density in air. This is identical to the parenthetical expression in the Richardson number (Step 2).

Initial conditions for releases of this type must be assumed. In this case, it is assumed that the gas released forms a hemisphere. An initial radius for the cylindrical heavy gas model is determined by equating the hemispherical and cylindrical volumes:

$$\frac{2}{3} \pi r^3 = \pi r^2 h$$

so that $h = \frac{2}{3}$ r. Then for the model

$$V_{o} = \frac{2}{3} \pi R_{o}^{3} \text{ and } R_{o} = \left(\frac{3 V_{o}}{2 \pi}\right)^{0.33}$$

The initial radius is:

$$R_{O} = \begin{bmatrix} 3 & (9 \text{ m}^{3}) \\ \hline 2 & 3.14 \end{bmatrix}^{0.33} = 1.62 \text{ m}$$

The entrained volume is:

$$V = 9.0 \text{ m}^3 \left(\frac{82 \text{ m}}{1.62 \text{ m}}\right)^{1.2} = 998.6 \text{ m}^3$$

 $V_T = 9.0 \text{ m}^3 + 998.6 \text{ m}^3 = 1.007.6 \text{ m}^3$

and:

$$H = \frac{1,007.6 \text{ m}^3}{3.14 (82 \text{ m})^2} = 0.05 \text{ m}$$

4) Instantaneous dispersion estimates are calculated for using a horizontal virtual point source approach for an area source since the cloud depth is small (i.e., x_z is insignificant):

$$x_{vy} = (23.26 \cdot 82 \text{ m})^{1.12} = 4721 \text{ m}$$
 $x_y = (100 \text{ m} + 4721 \text{ m}) = 4821 \text{ m}$

5) Dispersion parameters (Section 5.3.2) are obtained for F stability and used to determine concentration (Section 5.6.5):

$$\sigma_{y}$$
 (4821 m) = 38 m
 σ_{z} (100 m) = 0.8 m

$$C = \frac{0.127 \quad 50,000 \text{ g}}{(38 \text{ m})^{2} \quad 0.8 \text{ m}} = 5.5 \text{ g/m}^{3}$$

6.15 Liquid Release from a Pipe

Scenario: Concentrations are estimated from a transfer pipe failure between unsymmetrical dimethylhydrazine tanks resulting in an unconfined liquid pool.

<u>Discussion</u>: This scenario represents cases where liquid is released from pipes on the ground and, due to its low volatility, pooling occurs. Evaporation of the liquid results in formation of vapor for which continuous area source techniques can be used to simulate dispersion. It is assumed for screening that flow in the pipe is continuous and frictionless. The pool evaporation rate is assumed to reach a steady state after spreading such that the evaporation rate equals the pipe flow rate.

Source Parameters

- hydrazine (UDMH): density 0.786 g/cm³
 molecular weight 60.1 g/g-mole
 vapor pressure 19.88 x 10⁴ dynes/cm²
- flow rate $0.0001 \, \text{m}^3/\text{s}$
- ambient temperature 283 K
- minimum receptor distance 100 m

Sample Estimates

1) The path through calculations is presented in Section 4.15 as shown in Flowchart C-16. Estimates are calculated separately for pool spreading and evaporation and subsequent dispersion. The liquid release rate is given by:

$$q_1 = 0.786 \text{ g/cm}^3 (100 \text{ cm}^3/\text{s}) = 78.6 \text{ g/s}$$

2) Evaporation is calculated using an intermediate parameter of the evaporation model to determine the area at which the evaporation rate equals the release rate:

$$B = \frac{1.54 \times 10^{-4} (1 \text{ m/s})^{0.78} (60.1 \text{ g/g-mole})^{0.67} (19.88 \times 10^{4} \text{ dyne/cm}^{2})}{283 \text{ K}}$$

= 1.683

$$A = \left(\frac{78.6}{1.683}\right)^{1.06} = 58.8 \text{ m}^2$$

Since the spill is continuous and unconfined, no check is required for determining maximum area (Section 4.15).

3) The area of the evaporating pool is used in area source dispersion calculations using Flowchart D-4. The virtual source distance (Section 5.5.1) is obtained assuming a square pool:

$$W = \sqrt{58.8 \text{ m}^2} = 7.67 \text{ m}$$
 $\sigma_V = W/4.3 = 7.67 \text{ m}/4.3 = 1.78 \text{ m}$

From Figure 5-1, under stable conditions,:

$$x_v = 70 \text{ m}$$

and:

$$x_{y} = (100 + 70 \text{ m}) = 170 \text{ m}$$

for receptors at 100 m.

4) Dispersion parameters from Section 5.3.1 are used for F stability to determine concentration in Section 5.6.4 (with H = 0).

$$\sigma_{V} = (170 \text{ m}) = 7 \text{ m}$$

$$\sigma_z = (100 \text{ m}) = 2.3 \text{ m}$$

$$C = \frac{78.6 \text{ g/s}}{3.14 \text{ (7 m) } 2.3 \text{ m (1 m/s)}} = 1.55 \text{ g/m}^3$$

6.16 Low Volatility Liquid Releases from Tanks

Scenario: Maximum concentrations are estimated from a leak in an unpressurized tank containing unsymmetrical dimethylhydrazine (UDMH).

<u>Discussion</u>: This example represents a scenario where liquid is released from a storage tank and pools on the ground. Evaporation of the liquid results in a plume of vapor for which continuous area source techniques can be used to simulate dispersion.

Source Parameters

UDMH: - density - 0.786 g/cm³
- molecular weight - 60.1 g/g-mole
- vapor pressure - 19.88 x 10⁴ dynes/cm²
- tank pressure = atmospheric pressure

leak: - 100 cm below liquid level
- 8 cm² area

meteorology - wind speed - 2 m/s
- temperature - 283 deg. K
- stable (F)

receptor distance - 100 m (fenceline)
impoundment area - 2500 m²

Sample Estimates

The path through calculations is presented in Section 4.16 and Flowchart C-17. Estimates are calculated separately for release from the tank, pool spreading and evaporation and subsequent dispersion.

1) Using the release model, the liquid release rate is calculated as:

$$q_1 = 0.8 (8 \text{ cm}^2) 0.786 \text{ g/cm}^3 \sqrt{1960 (100 \text{ cm}) + 0}$$

= 2227 g/s

2) Evaporation is calculated using an intermediate parameter of the evaporation model to determine the area at which the evaporation rate equals the release rate (as described in Section 4.15):

$$B = \frac{1.54 \times 10^{-4} (1 \text{ m/s})^{0.78} (60.1 \text{ g/g-mole})^{0.67} (1.988 \times 10^{5} \text{ dyne/cm}^{2})}{283 \text{ K}}$$

= 1.683

$$A = \left(\frac{2227}{1.683}\right)^{1.06} = 2037 \text{ m}^2$$

The area of the evaporating pool is the smaller of the impoundment area (2500 m^2) and the area at which evaporation across the pool equals flow into the pool (2037 m^2). Therefore, the vapor emission rate equals the liquid release rate:

$$q_v = q_1 = 2227 \text{ g/s}$$

Alternatively, q, can be calculated as in Section 4.15.

3) Dispersion calculations follow using Flowchart D-4. The virtual source distance using the width of a square impoundment is (Section 5.5.1):

$$W = \sqrt{2037} = 45.1 \text{ m}$$
 $\sigma_{VO} = W/4.3 = 45.1 \text{ m}/4.3 = 10.5 \text{ m}$

From Figure 5-1, under stable (F) conditions,:

$$x_{xy} = 280 \text{ m}$$

and:
$$x_y = (280 + 100 \text{ m}) = 380 \text{ m}$$

4) Dispersion parameters are determined for stability F in Section 5.3.1. Concentrations are calculated using Section 5.6.4 (with H = 0):

$$\sigma_{V}$$
 (380 m) = 14 m

$$\sigma_{z}$$
 (100 m) = 2.3 m

$$C = \frac{2227 \text{ g/s}}{\pi \text{ (14 m) (2.3 m) (1 m/s)}} = 22.01 \text{ g/m}^3$$

6.17 High Volatility Liquid Release from a Pipe

Scenario: Aminomethane liquid is released from a small pipe, and a concentration estimate is required for a site with a minimum receptor distance of 100 m downwind.

<u>Discussion</u>: The high volatility liquid release is intended to represent calculations for materials which when released immediately volatilize and are airborne. Estimates of the liquid release rate are required, but the material can be considered gaseous at the source. A continuous dispersion model can then be used to estimate downwind dispersion. For pipe releases, the screening technique is to assume that the volume rate of release equals the emission to the atmosphere and is determined by the flow volume in the pipe.

Source Parameters

- liquid characteristics density 0.69 g/cm³
 molecular weight 31 g/g-mole
 boiling point -6.3 deg. C
- liquid mass flow rate 9.8 g/s
- wind speed 1 m/s
- ambient temperature 283 K

Sample Estimates

1) A technique for estimating emissions is provided in Section 4.17 and Flowchart C-19. The release rate is assumed to equal the pipe flow rate:

$$q_1 = 9.8 \text{ g/s}$$

In this example, it is assumed that aminomethane has a sufficiently high vapor pressure that evaporation from a small leak is instantaneous and no pooling results. Such an instantaneous vaporization results in a vapor cloud which is roughly at the boiling point of the liquid. This assumption could be checked using techniques presented in Section 4.15.

2) Simulations of dispersion follow Flowchart D-1 for passive continuous releases. A check of plume density shows that the release at the boiling temperature is slightly more dense than air (Section 5.1.2). Calculation of the Richardson number as a density check requires a determination of the volume release rate using the molar volume and molecular weight:

$$V = \frac{9.8 \text{ g/s}}{31 \text{ g/g-mole}} \frac{(0.0224 \text{ m}^3)}{\text{g-mole}} \frac{(267 \text{ K})}{(273 \text{ K})}$$
$$= 6.9 \times 10^{-3} \text{ m}^3/\text{s}$$

and effective diameter:

$$d = \sqrt{\frac{4 (6.9 \times 10^{-3})}{3.14 (1 \text{ m/s})}} = 0.094 \text{ m}$$

The Richardson number is given by:

Ri = 2722
$$\left(\frac{(31 \text{ g/g-mole}) (283 \text{ K})}{28.9 \text{ g/g-mole} (267 \text{ K})} - 1\right) \frac{0.0069 \text{ m}^3/\text{s}}{(1 \text{ m/s})^3 (0.094 \text{ m})}$$

= 27

A value of less than 30 confirms that the release is essentially passive.

- 3) Since, in this scenario, no pooling occurs, point source dispersion calculations (Flowchart D-2) can be used to calculate concentration. No information is available on the setting of the leak relative to the tank dimensions or other structures so that the estimate cannot evaluate the effects of downwash. In the absence of this information, the most conservative assumption is to consider the source a continuous ground level point source. In addition, because the release is not heated, no buoyancy plume rise occurs (Section 5.2.3).
- 4) Point source dispersion calculations (Flowchart D-3) begin with specification of dispersion parameters (Section 5.3.1) for F stability:

$$\sigma_{y}$$
 (100 m) = 4 m
 σ_{z} (100 m) = 2.3 m

5) Because there is no plume rise, buoyancy induced dispersion (Section 5.4) does not apply. Concentration is estimated by (Section 5.6.4 with H=0):

$$C = \frac{9.8 \text{ g/s}}{3.14 \text{ (4 m) (2.3 m) 1 m/s}} = 0.339 \text{ g/m}^3$$

6.18 High Volatility Liquid Releases from Tanks

Scenario: Aminomethane liquid is released from a minor tank leak and a maximum concentration estimate is required for a fenceline receptor 100 m downwind.

<u>Discussion</u>: The high volatility liquid release is intended to represent calculations for materials which, when released, immediately evaporate (no pooling results). In this example, it is assumed that aminomethane has a sufficiently high vapor pressure so that evaporation from a small leak is instantaneous and no pooling results. Estimates of the liquid release rate are required, but the material can be considered gaseous at the source. This scenario shares many of the calculations found in example Section 6.17. Differences lie only in the release and emission calculations. In both, steady-state release estimates are used in a dispersion model. In a refined analysis, the examples would show different release rates as pressure in the transfer line or tank is reduced. A continuous dispersion model can then be used to estimate downwind dispersion.

Source Parameters

```
liquid characteristics - density - 0.69 g/cm<sup>3</sup>
- molecular weight - 31 g/g-mole
- boiling point - -6.3 deg. C (267 deg. K)
tank pressure - 2.03 x 10<sup>6</sup> dynes/cm<sup>2</sup>
atmospheric pressure - 1.01 x 10<sup>6</sup> dynes/cm<sup>2</sup>
ambient temperature - 283 deg. K
release depth - 100 cm below liquid level
release area - 0.01 cm<sup>2</sup>
wind speed - 2 m/s
stability - neutral
```

Sample Estimates

1) Techniques to estimate emissions are provided in Section 4.18 and Flowchart C-19. The release rate is calculated by:

$$q_1 = 0.8(0.01 \text{ cm}^2) \ 0.69 \text{ g/cm}^3 \cdot$$

$$\sqrt{\frac{1960 \ (100 \text{ cm}) + 2(2.03 \times 10^6 - 1.01 \times 10^6)}{0.69 \text{ g/cm}^3}} \text{ dynes/cm}^2$$

$$= 9.8 \text{ g/s}$$

2) Simulations of dispersion follow Flowchart D-1 for continuous releases. No information is available on the location of the leak relative to the tank dimensions or other structures so that the estimate cannot evaluate the effects of downwash. In the absence of this information, the most conservative assumption is to consider the source a continuous ground level point source.

A check of plume density shows that the release (31 g/g-mole) at the boiling temperature is slightly more dense than air (28.9 g/g-mole). Thus, a check of the Richardson number (Section 5.1.2) must be made.

The volume rate is calculated at ambient temperature using the molar weight and gas molar volume at ambient temperature:

$$V = \frac{9.8 \text{ g/s}}{31 \text{ g/g-mole}} \left(0.0224 \frac{\text{m}^3}{\text{g-mole}} \right) \left(\frac{267 \text{ K}}{273 \text{ K}} \right)$$
$$= 6.9 \times 10^{-3} \text{ m}^3/\text{s}$$

An equivalent diameter is calculated:

$$d = \sqrt{\frac{4 \text{ (6.9 x } 10^{-3})}{\text{(3.14) 1 m/s}}} = 0.094$$

Then,

Ri = 2722
$$\left(\frac{\text{(31 g/g-mole)(283 deg. K)}}{28.9 \text{ g/g-mole (267 deg. K)}} - 1\right) \frac{0.0069 \text{ m}^3/\text{s}}{(1 \text{ m/s})^3 0.094 \text{ m}} = 27$$

Since Ri < 30, the release is essentially passive.

3) As with Example 6.17, no downwash, plume rise, or buoyancy induced dispersion apply. Therefore, once dispersion parameters are determined (Flowchart D-3, Section 5.3.1), receptor concentration can be calculated (Section 5.6.4):

$$\sigma_v$$
 (100 m) = 4 m

$$\sigma_z$$
 (100 m) = 2.3 m

$$C = \frac{9.8 \text{ g/s}}{3.14 (2.3 \text{ m}) (4 \text{ m}) 1 \text{ m/s}} = 0.339 \text{ g/m}^3$$

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APPENDIX A EMISSION FACTORS

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EMISSION FACTORS

One alternative for estimating air toxic emissions from sources is through the use of emission factors. Emission factors have been developed for a number of processes and pollutants. Emission factors provide an estimate of emissions as a function of source activity such as process rate or some other operating parameter. Emission factors are intended to be used for making preliminary estimates of toxic air emissions. As such, they represent generic factors whose applicability to a specific source may be questionable. These factors will not likely provide exact estimates of emissions from any particular source. The source of an emission factor must be carefully evaluated to determine whether it is applicable to a particular facility. Emission factors are available for both area and point sources. Some sources of emission factors applicable to air toxics emissions are presented below.

1) U.S. Environmental Protection Agency. <u>Locating and Estimating Air</u> Emissions from Sources of (Substance). EPA 450/4-84-007a-q.

EPA has underway a program to compile and publish emission factors for various air toxics. To date, sixteen reports have been published as part of this program. The substances covered by this series include: acrylonitrile, carbon tetrachloride, chloroform, ethylene dichloride, formaldehyde, nickel, chromium, manganese, phosgene, epichlorohydrin, vinylidene chloride, ethylene oxide, chlorobenzenes, PCBs, POM, and benzene.

2) U.S. Environmental Protection Agency. <u>Survey of (Substance) Emission</u> Sources.

A second series of reports on specific air toxics has been developed by EPA as part of the National Emissions Standards For Hazardous Air Pollutants (NESHAPS) program. The substances covered by this series include: trichloroethylene (EPA 450/3-85-021), perchloroethylene (EPA 450/3-85-017), ethylene oxide (EPA 450/3-85-014), chloroform (EPA 450/3-85-026), ethylene dichloride (EPA 450/3-84-018), methylene chloride (EPA 450/3-85-015), and carbon tetrachloride (EPA 450/3-85-018).

3) U.S. Environmental Protection Agency. <u>Preliminary Compilation of Air Pollutant Emission Factors for Selected Air Toxic Compounds</u>. <u>EPA-450/4-86-010a</u>, 1987.

This preliminary report presents emission factors of air toxic pollutants for a variety of sources with varying activity levels. This listing gives little technical detail concerning the derivations or applicability of any of the factors therein. This preliminary report is currently being updated and expanded and a data management system is being developed to allow for easy access of the factors. The updated factors are associated with pollutant names and CAS numbers, process descriptions and SIC codes, emission source descriptions and SCC codes, notes on the derivation of the factors and on control measures associated with the factors, and references. The emission factors can be used to obtain quick, rough estimates of air toxic emissions. More detailed data on the emission sources can be obtained from the Notes and References Sections listed in the emission factor tables. The primary limitation of using just the emission factors listed in this compilation is that their accuracy in application to a given source is not shown. More accurate emissions estimates may require evaluation of the application of available test data to specific source characteristics.

4) U.S. Environmental Protection Agency. Compilation of Air Pollutant Emission Factors, Fourth Edition. AP-42, September 1985. Air Emissions Species Manual, Volume I, Volatile Organic Compound Species Profiles. EPA 450/2-88-003a, 1988. Air Emissions Species Manual, Volume II, Particulate Matter Species Profiles. EPA-450/2-88-003b, 1988.

Another tool for estimating air toxic emissions involves the use of VOC/PM factors presented in AP-42 and species profiles presented in Volumes I and II of the Air Emissions Species Manual. AP-42 contains emission factors for total VOC and PM rather than for a single chemical compound. These factors can be used with profiles contained in the Species Manual to estimate releases of specific toxic compounds based on the total amount of VOC or PM released from a source. The Species Manual shows the percent by weight and percent by volume of specific chemicals in emissions from specific chemicals in emissions from specific processes. The VOC profiles were obtained from the 1980 VOC Data Manual, new VOC profiles developed from readily available existing data, and new VOC profiles developed from original data as part of the VOC speciation field sampling program. The PM profiles were obtained from the 1984 Source Composition Library and from the literature. In addition to the VOC and PM profiles, profile assignments linking the profiles to source categories are presented in the Species Manual. Species profiles for VOCs and PM are developed from generic sources and may not be representative of emissions from an individual facility.

5) U.S. Environmental Protection Agency. <u>Fugitive Emission Sources of Organic Compounds - Additional Information on Emissions, Emission Reductions</u>, and Costs. <u>EPA-450/3-82-010</u>, 1982.

This document contains the data and methodologies which EPA believes most accurately characterize average synthetic organic chemical manufacturing industry equipment leak emission rates of VOC, effectiveness of control techniques, and control costs for selected equipment used in the processing of organic chemicals. The emission factors (on Page 1-4) can be used to estimate VOC emissions from any industrial plant which has the selected equipment and handles organic chemicals.

APPENDIX B

GLOSSARY

APPENDIX B

GLOSSARY

Accident - In this workbook, an unplanned release event not considered in the design of a facility; a major or catastrophic release (e.g., release from a tank rupture disk).

Boiling - Vaporization resulting from heat transfer to liquids with boiling temperatures below ambient or spill surface temperatures.

Cavity - An aerodynamic recirculation zone formed in the lee of an obstruction (e.g., building) in a wind field.

Continuous Release - A release for which the discharge rate is not time varying or instantaneous; a dispersing plume for which sampling at a receptor observes little or no variability due to a time change of emissions (see instantaneous).

Dense gas - Gas mixtures that are denser than the surrounding air. A dense gas may rise at first due to its initial upward momentum from a stack, but then sinks due to its excess density. In the context of this workbook, a release can result in dense gas effects if its release Richardson number is > 30.

Depositing - Removal from a plume of gases or particles by chemical or physical interactions with surfaces or by precipitation.

Emissions - A release of gas, aerosols or particulate matter to the atmosphere; a gaseous release is an emission while a liquid release must evaporate before being emitted.

Evaporation - Vaporization resulting from mass transfer; i.e., turbulent interactions between the atmosphere and the liquid surface.

Fugitive emissions - Emissions resulting from a source for which quantifying release parameters, emission rates, and locations is difficult. Emissions estimates may result from emission factors or mass balance calculations and typically represent a number of small disperse emission sources at a facility.

Instantaneous release - 1) For a liquid, a release which occurs within a very short time. An instantaneous liquid release may result in formation of an instantaneous gaseous or two-phase cloud if the liquid is highly volatile or a pool from which emissions may be continuous or highly time dependent. 2) For a gas, a release is considered instantaneous for modeling if:

- the travel time to a receptor is long relative to the length of the
- the averaging or sampling time is long relative to the release time

An instantaneous model is used if the concentration estimate at a receptor is significantly affected by the upwind and or downwind edge of the cloud. For this workbook, releases of less than five minutes duration are arbitrarily considered instantaneous.

Neutral - 1) A stability class in which mixing is controlled by mechanical turbulence; 2) A passive or tracer release, see passive release.

Passive release - Emissions to the atmosphere which disperse as a tracer, i.e., as a massless point in space which in no way influences the environment in which it disperses; sometimes called a neutral buoyancy release as opposed to releases for which buoyancy is important in dispersion.

Pool, pooling - Accumulation of released liquid in a puddle on a surface; pools may be unconfined or spreading, confined by a berm or dike or steady-state for which evaporation equals input to the pool and spreading is halted.

Reactive - Dispersing pollutants which chemically interact with surfaces or other chemicals resulting in a transformation to another chemical. Reactions are important in estimating pollutant losses or formation as well as in estimating energy balances in plumes.

Release - Chemicals or pollutants leaving containment, stacks or vents.

Slumping - Initial spread of a dense gas characterized by vertical sinking and horizontal spreading resulting from (negative) buoyant or gravitational forces acting on the cloud.

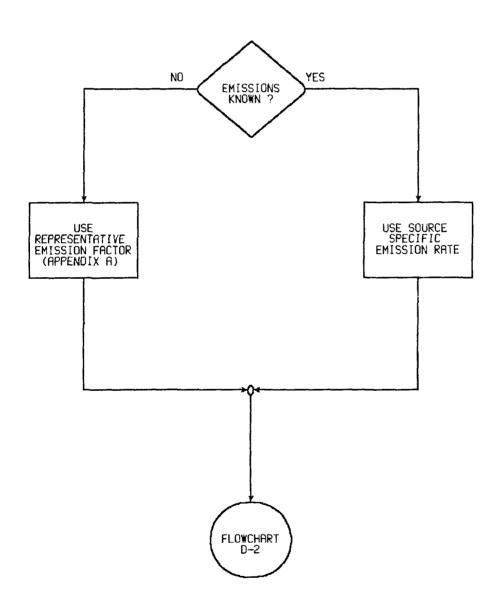
Two-phase release - Releases consisting of a vapor and suspended liquid droplets resulting from the violent flash vaporization of superheated liquids as they rapidly depressurize.

Volatile - A liquid subject to high vaporization due to its high vapor pressure. In this workbook, the term high volatility is intended to represent liquids that pool after release requiring an evaporation model to simulate emissions. If a doubt exists, the liquid can be simulated using an evaporation model. An assumption of rapid evaporation of a high volatility liquid is a conservative assumption.

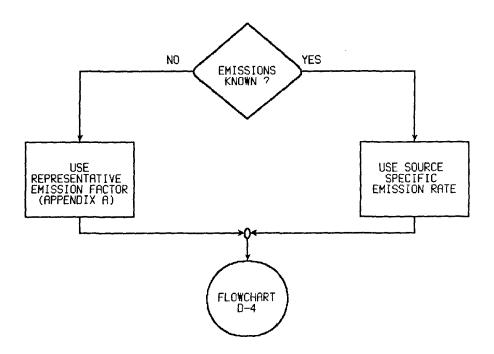
Wake - The entire zone of wind field disturbance caused by an obstruction in the flow.

APPENDIX C FLOWCHARTS FOR WORKBOOK SCENARIOS

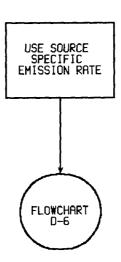
FLOWCHART C-1
CONTINUOUS PARTICULATE EMISSIONS FROM STACKS



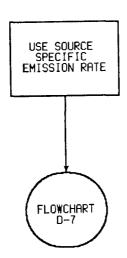
FLOWCHART C-2
CONTINUOUS FUGITIVE DUST EMISSIONS



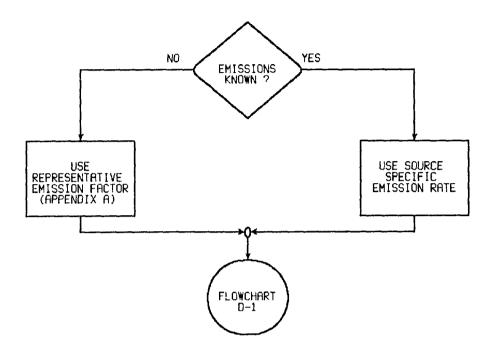
FLOWCHART C-3 INSTANTANEOUS PARTICULATE EMISSIONS FROM DUCT FAILURES



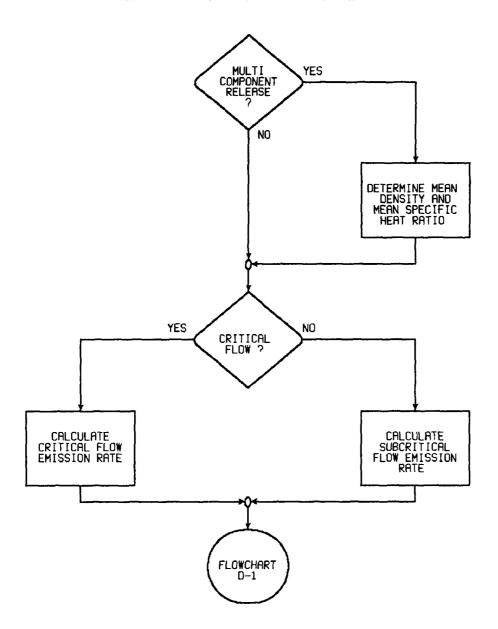
FLOWCHART C-4 CONTINUOUS FLARE EMISSIONS



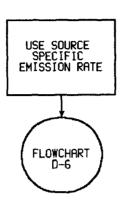
FLOWCHART C-5
CONTINUOUS GASEOUS EMISSIONS FROM STACKS



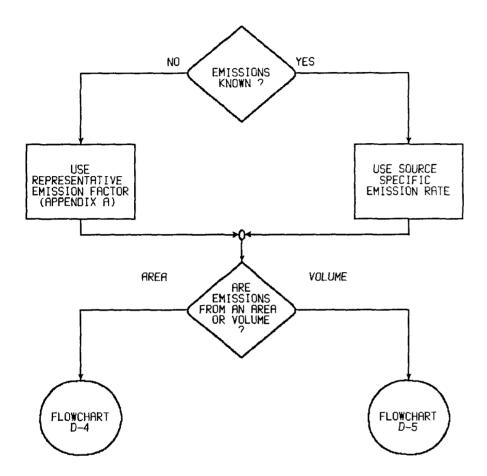
FLOWCHART C-6
CONTINUOUS GASEOUS LEAKS FROM TANKS/PIPES



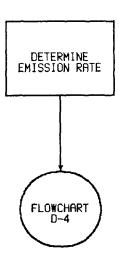
FLOWCHART C-7
INSTANTANEOUS GASEOUS EMISSIONS FROM STACKS/VENTS



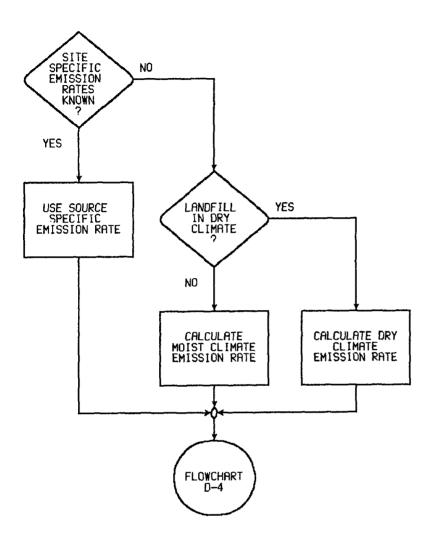
FLOWCHART C-8
MULTIPLE FUGITIVE CONTINUOUS GASEOUS EMISSIONS



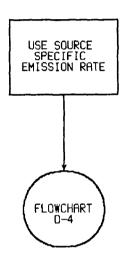
FLOWCHART C-9
CONTINUOUS GASEOUS EMISSIONS FROM LAND TREATMENT



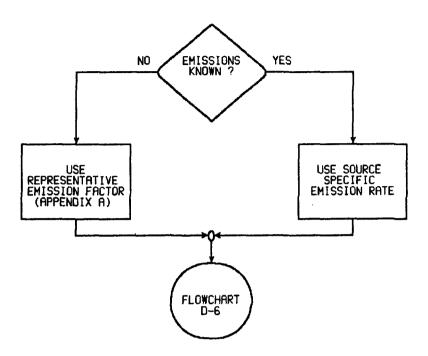
FLOWCHART C-10
CONTINUOUS GASEOUS EMISSIONS FROM LANDFILLS



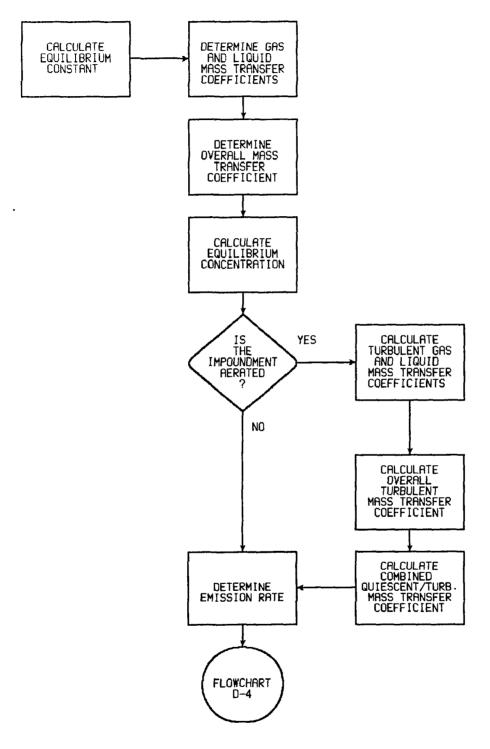
FLOWCHART C-11 PESTICIDE/HERBICIDE VOLATILIZATION



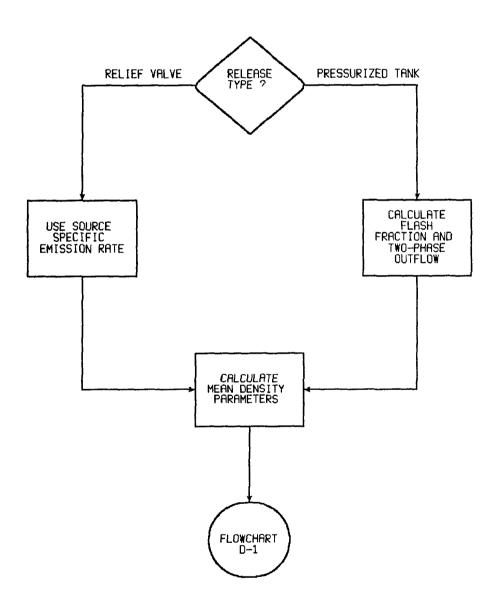
FLOWCHART C-12
INSTANTANEOUS GASEOUS EMISSIONS DUE TO EQUIPMENT OPENINGS



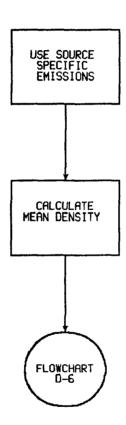
FLOWCHART C-13
SURFACE IMPOUNDMENT EMISSIONS



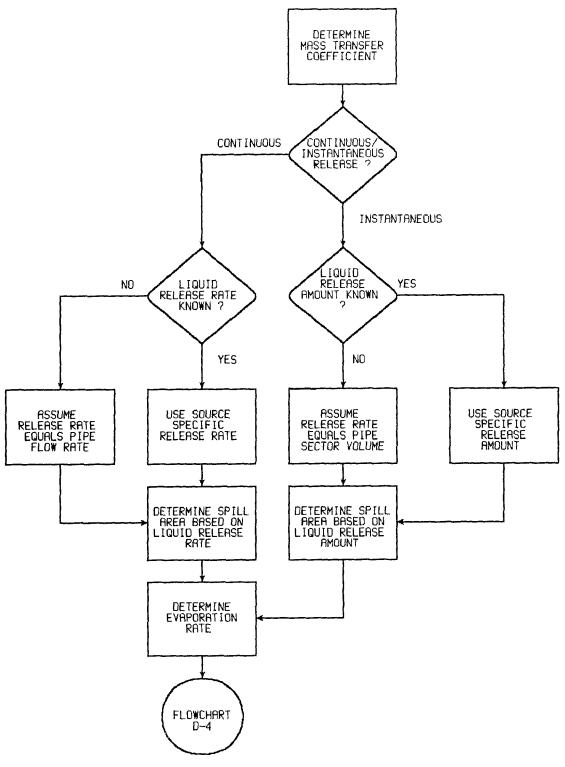
FLOWCHART C-14 CONTINOUS RELIEF VALVE DISCHARGE (TWO-PHASE)



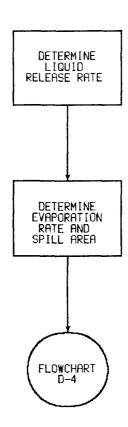
FLOWCHART C-15 INSTANTANEOUS RELIEF VALVE DISCHARGE (TWO-PHASE)



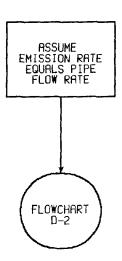
FLOWCHART C-16
EMISSIONS DUE TO LOW VOLATILITY LIQUID LEAKS FROM PIPES



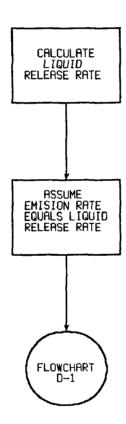
$\label{eq:flowchart} \mbox{${\it E}$-17$}$ EMISSIONS DUE TO LEAKS OF LOW VOLATILITY LIQUIDS FROM TANKS



FLOWCHART C-18 EMISSIONS DUE TO LEAKS OF HIGH VOLATILITY LIQUIDS FROM PIPES

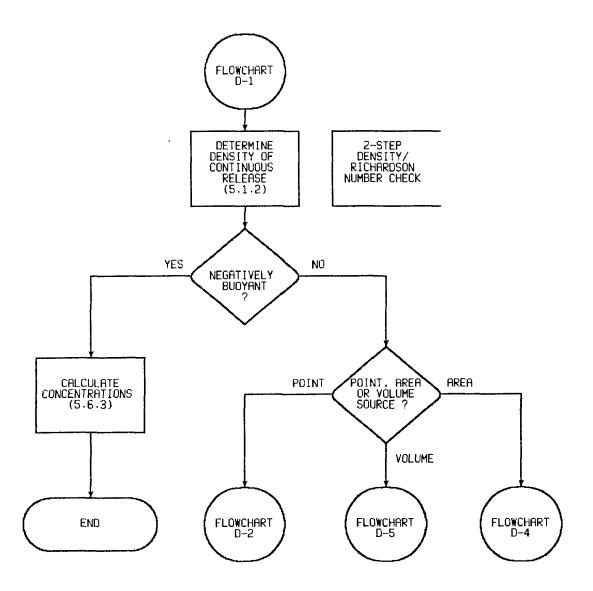


FLOWCHART C-19 EMISSIONS DUE TO LEAKS OF HIGH VOLATILITY LIQUIDS FROM TANKS

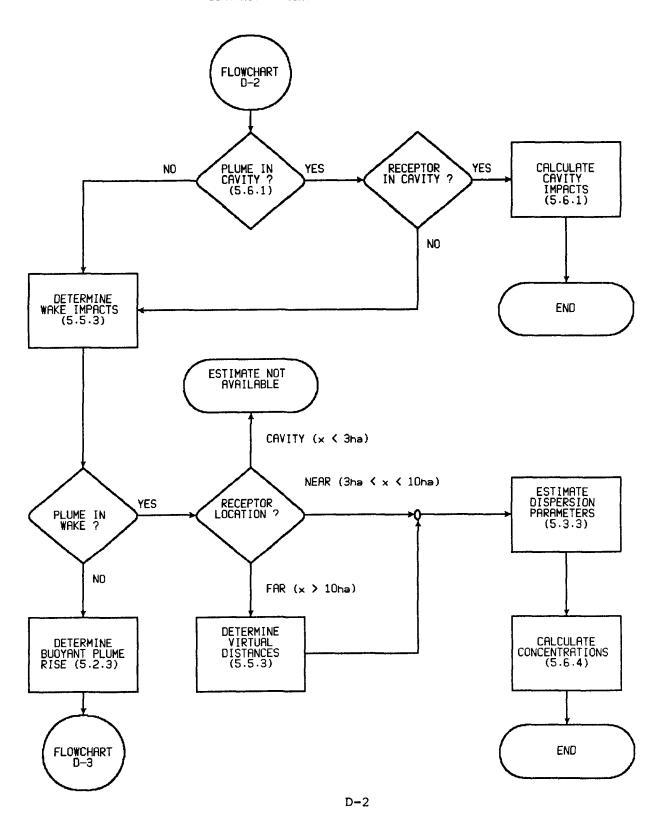


APPENDIX D FLOWCHARTS FOR DISPERSION CALCULATIONS

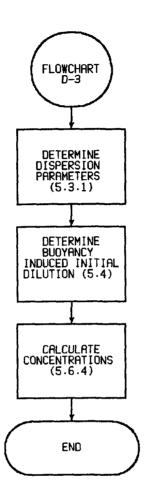
FLOWCHART D-1
DETERMINATION OF DISPERSION CLASS FOR CONTINUOUS SOURCES



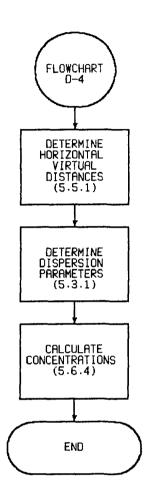
FLOWCHART D-2
CONTINUOUS POINT SOURCE CALCULATIONS



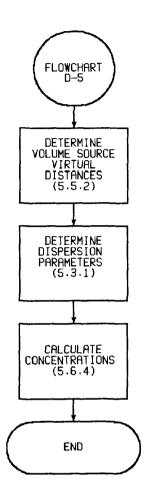
FLOWCHART D-3
CONTINUOUS POINT SOURCE DISPERSION CALCULATIONS



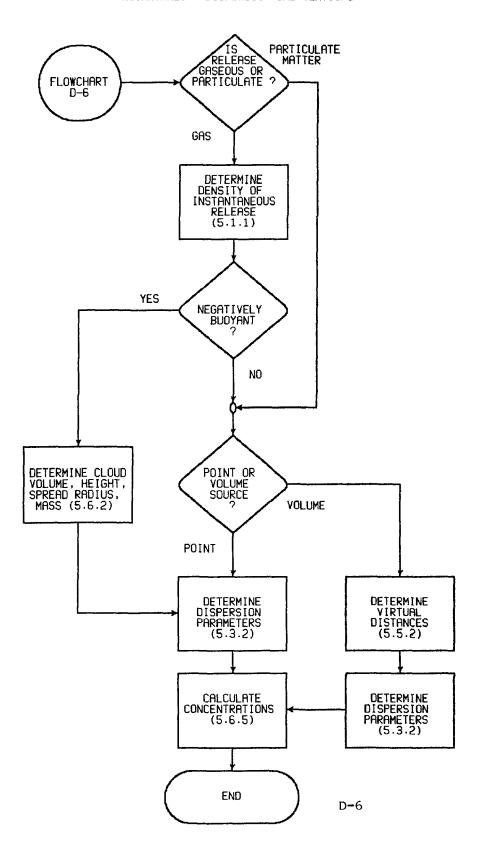
FLOWCHART D-4
CONTINUOUS AREA SOURCE DISPERSION CALCULATIONS



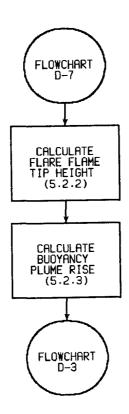
FLOWCHART D-5
CONTINUOUS VOLUME SOURCE DISPERSION CALCULATIONS



FLOWCHART D-6
INSTANTANEOUS DISPERSION CALCULATIONS



FLOWCHART D-7
CONTINUOUS FLARE CALCULATIONS



APPENDIX E

AVERAGING PERIOD OF CONCENTRATION ESTIMATES

APPENDIX E

AVERAGING PERIOD OF CONCENTRATION ESTIMATES

The purpose of this appendix is to provide some simplified techniques for concentration averaging from instantaneous and continuous equations provided in the workbook. Methods presented are applicable to ground-level and elevated emissions of passive gases and particulate matter.

Instantaneous Estimates

Methods provided for instantaneous concentration estimates (i.e., puff releases with a duration of 5 minutes or less) in Section 5.6.5 represent peak concentrations at the centroid of an expanding puff transported in the wind. Petersen (1982) provides equations for estimating peak average concentrations over time periods of up to one hour. The method is as follows:

$$C(mean) = C(instantaneous) \times F$$

where the correction factor (F) represents the mean height of the area of the Gaussian puff which traverses a receptor in the sampling time (τ). It is given by:

$$F = (A - 0.5)/(0.3989 N)$$

where:

A = the area under the Gaussian distribution within N standard deviations, as found in Figure E-1

N = the number of standard deviations from the peak defined as:

$$N = \frac{\tau u}{2\sigma_r}$$

 τ - averaging time in seconds

u - transport wind speed (m/s)

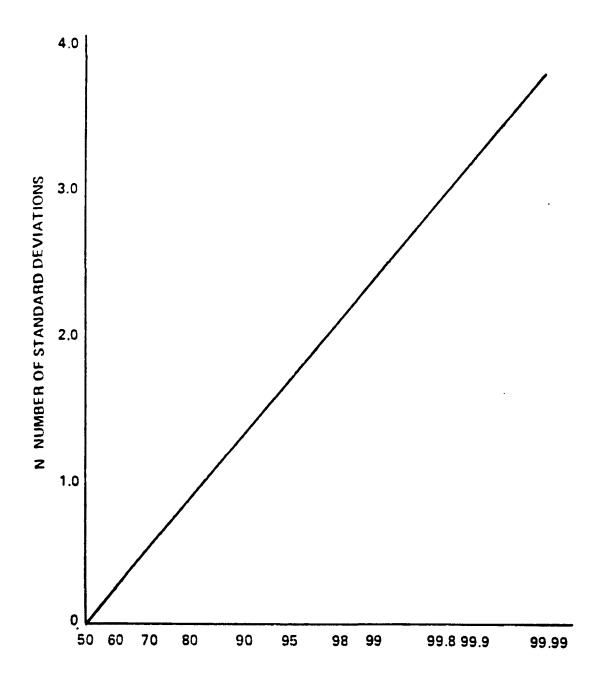
 σ_{r} - instantaneous horizontal plume dispersion parameter at the receptor distance (m) (from Figure 5-4)

• Continuous Estimates

To obtain the estimate of the maximum concentration for a longer averaging time, multiply the 1-hour maximum concentration by the given factor:

0.9 (±0.1)
$0.7 (\pm 0.2)$
$0.4 (\pm 0.2)$

FIGURE E-1
AREA UNDER NORMAL CURVE



The numbers in parentheses are recommended limits to which one may diverge from the multiplying factors representing the general case. For example, if aerodynamic downwash or terrain is a problem at the facility, or if the release height is very low, it may be appropriate to increase the factors up to the limits specified in parentheses. Conversely, if the stack is relatively tall and there are no terrain or downwash problems, it may be appropriate to decrease the factors. For averaging times in between the values listed above, use the multiplying factor for the shorter averaging time. For example, if a 4-hour average concentration is needed, use the multiplying factor for the 3-hour averaging time (0.9).

To obtain the estimated maximum concentration for a shorter averaging time than 1-hour, use the 1-hour maximum concentration for any desired averaging time between 30 and 60 minutes. For averaging times less than 30 minutes, a specific procedure can not be recommended.

To obtain the estimate time, C_t , he is horter arranging time than I have adjust the 1-hour trax conce by the following respect to $C_t = C_{1-hour} \left(60 \text{ min}/t \right)^{0.2}$ where:

t - averiging period of interest (less than 60 mm)

APPENDIX F

SELECTED CONVERSION FACTORS

APPENDIX F

SELECTED CONVERSION FACTORS

Pressure

1 ATM = 1.013 x 10^6 dynes/cm² 1 millibar = 1000 dynes/cm² 1 mm Hg = 1333.224 dynes/cm² 1 lb/in² = 68,947.6 dynes/cm² 1 in. Hg = 33,863.9 dynes/cm² 1 Pascal = 10 dynes/cm²

Volume

 $1 m^3 = 10^6 cm^3$ $1 m^3 = 10^3 liters$ 1 cu ft = 28.317 liters $1 liter = 10^3 cm^3$ $1 m^3 = 35.315 cu feet$ $1 gal = 3.785 cm^3$

Mass Release Rate

l g/s = 7.9367 lb/hr l t/yr = 2.8766 x 10^{-2} g/s lt/day = 10.500 g/s

Concentration

Conversions with parts per million by volume

$$\mu g/m^3 = (ppm) 40.87 \text{ MW} \left[\frac{P}{Po} \left(\frac{To}{T} \right) \right]$$

$$ppm = (\mu g/m^3) \frac{0.02447}{MW} \left[\frac{Po}{P} \left(\frac{T}{To} \right) \right]$$

Energy

1 cal (g) = 3.9685×10^{-3} BTU 1 BTU = 251.634 cal 1 BTU = 1.0543×10^{10} ergs 1 BTU = 1054 Joules - (N - m)

Heat Rate

 $1 \text{ cal/s} = 1.102 \times 10^{-6} \text{ BTU/h}$

Flow

 $1 m^3/h = 3600 m^3/s$

Area

 $1 m^2 = 10^4 cm^2$ $1 ft^2 = 0.0929 m^2$ $1 hectare = 10^4 m^2$ $1 acre = 4046.86 m^2$



APPENDIX G

CALCULATIONAL METHODS FOR DISPERSION PARAMETERS

APPENDIX G

CALCULATIONAL METHODS FOR DISPERSION PARAMETERS

Dispersion parameters presented graphically in Section 5.3.1 and 5.3.2 are statistical fits to observed experimental data. Dispersion parameters may be derived from these figures or from equations presented in this appendix.

Instantaneous dispersion parameters are derived from quasi-instantaneous releases (Slade, 1968). The parameters are of the form:

$$\sigma = a x^b$$

where x is the downwind distance in meters and the coefficients are given by:

STABILITY	HORIZONTAL		VERT	CICAL	
	a	b	a	b	
Unstable (A-C)	0.14	0.92	0.53	0.73	
Neutral (D)	0.06	0.92	0.15	0.70	
Stable (E-F)	0.02	0.89	0.05	0.61	

Pasquill-Gifford dispersion parameters for continuous sources can be calculated using downwind distance in kilometers using Figures 5-1 and 5-2 or techniques from ISC (EPA, 1987c) given in Tables G-1 and G-2:

TABLE G-1 $\label{eq:continuous} \mbox{PARAMETERS USED TO CALCULATE PASQUILL-GIFFORD } \sigma_{\mbox{\bf y}}$

Pasquill Stability Category	σ_{y} (meters) = 465	
	С	đ
A	24.17	2.53
В	18.33	1.81
C	12.50	1.09
D	8.33	0.72
E	6.25	0.54
F	4.17	0.36

^{*} Where $\sigma_{\mbox{\bf y}}$ is in meters and x is in kilometers

TABLE G-2 $\label{eq:g-2} \mbox{PARAMETERS USED TO CALCULATE PASQUILL-GIFFORD } \sigma_{\mathbf{z}}$

Pasquill		$\sigma_{_{m{Z}}}$ (meter	$(xs) = a x^b$
Stability Category	x (km)	a	b
A*	<.10	122.800	0.94470
	0.10 - 0.15	158.080	1.05420
	0.16 - 0.20	170.220	1.09320
	0.21 - 0.25	179.520	1.12620
	0.26 - 0.30	217.410	1.26440
	0.31 - 0.40	258.890	1.40940
	0.41 - 0.50	346.750	1.72830
	0.51 - 3.11	453.850	2.11660
	>3.11	**	**
B *	<.20	90.673	0.93198
	0.21 - 0.40	98.483	0.98332
	>0.40	109.300	1.09710
C*	All	61.141	0.91465
D*	<.30	34.459	0.86974
	0.31 - 1.00	32.093	0.81066
	1.01 - 3.00	32.093	0.64403
	3.01 - 10.00	33.504	0.60486
	10.01 - 30.00	36.650	0.56589
	>30.00	44.053	0.51179

^{*} If the calculated value of $\sigma_{\mathbf{z}}$ exceeds 5000 m, $\sigma_{\mathbf{z}}$ is set to 5000 m.

^{**} is equal to 5000 m.

TABLE G-2 $({\tt Continued}) \\$ PARAMETERS USED TO CALCULATE PASQUILL-GIFFORD $\sigma_{\bf z}$

Pasquill		$\sigma_{\mathbf{z}}$ (mete	$rs) = a x^b$
Stability Category	x (km)	a	þ
E	<.10	24.260	0.83660
	0.10 - 0.30	23.331	0.81956
	0.31 - 1.00	21.628	0.75660
	1.01 - 2.00	21.628	0.63077
	2.01 - 4.00	22.534	0.57154
	4.01 - 10.00	24.703	0.50527
	10.01 - 20.00	26.970	0.46713
	20.01 - 40.00	35.420	0.37615
	>40.00	47.618	0.29592
F	<.20	15.209	0.81558
	0.21 - 0.70	14.457	0.78407
	0.71 - 1.00	13.953	0.68465
	1.01 - 2.00	13.953	0.63227
	2.01 - 3.00	14.823	0.54503
	3.01 - 7.00	16.187	0.46490
	7.01 - 15.00	17.836	0.41507
	15.01 - 30.00	22.651	0.32681
	30.01 - 60.00	27.074	0.27436
	>60.00	34.219	0.21716

ADDENDUM

"A Workbook of Screening Techniques for Assessing Impacts of Toxic Air Pollutants" -- September 1988

- Page 1-1: The title and reference of the publication "Procedures for Evaluating Impact of Stationary Sources" (1988b) is now "Screening Procedures for Estimating the Air Quality Impact of Stationary Sources," Brode, 1988. EPA-450/4-88-010.
- Page 2-9: Table 2-2 is taken from Appendix A of Brode (1988) referenced above.
- Page 6-17: Model output shown is based on a preliminary version of RVD run on 8/16/88. Results may differ from those obtained when using the final version of RVD.
- Page 6-41: Same comment about RVD model output as above.
- Page R-2: The reference "U.S. Environmental Protection Agency, 1988b: Procedures of Evaluating Impact of Stationary Sources," Draft Report, September 1988 is now "Brode, R. W., 1988: Screening Procedures for Estimating the Air Quality Impact of Stationary Sources," Draft for public comment, August 1988. EPA-450/4-88-010.
- Page E-3: Delete the last paragraph. Replace with the following paragraph:

To obtain the estimated maximum concentration, C_t , for a shorter averaging time than 1 hour adjust the 1-hour maximum concentration by the following ratio:

$$C_t = C_{1-hour} (60 \text{ min/t})^{0.2}$$

where:

t - averaging period of interest (less
 than 60 minutes)